U.S. DEPARTMENT OF COMMERCE
PATENT AND TRADEMARK OFFICE

ONLINE SEARCH REQUEST FORM

2-355

USER DAFOW SERIAL NUMBER 244863

ART UNIT 124 PHONE X4710 DATE 3/21/95

Please give a detailed statement of requirements. Describe as specifically as possible the subject matter to be searched. Define any terms that may have special meaning. Give examples or relevant citations, authors, or keywords, if known.

You may include a copy of the broadest and or relevant claim(s).

Z - R - A - R' - Y

Z,Y = cyclic polyamine having 9-20 ring members & 3-6 N atoms ...

R, R' = -C-

A = aromatic or heterocyclic group

OR then:

N - R - A - R' - N

cyclic atoms in 9-20 member rings

Bruckner Gary

STAFF USE ONLY

COMPLETED 3-25-95

SEARCHER JUNAI DANTZLER

ONLINE TIME 62 (in minutes) TOTAL TIME 82

DATABASES 3

SYSTEMS
- X CAS ONLINE
- ___ DARC/QUESTEL
- ___ DIALOG
- ___ SDC
- ___ OTHER

=>
=> d his l7-

(FILE 'CA' ENTERED AT 13:36:51 ON 25 MAR 95)
L7 37 S BRIDGER G?/AU
L8 2 S L7 AND (HIV OR AIDS OR HTLV OR IMMUNODEFIC?)
L9 1 S L7 AND CYCLIC
L10 2 S L8 OR L9

AUTHOR

=> d all

L10 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS
AN 120:30786 CA
TI Linked heterocyclic polyamines with activity against **HIV**
IN **Bridger, Gary James**; Padmanabhan, Sreenivasan; Skerlj, Renato Tony; Thornton, David Michael
PA Johnson Matthey P.L.C., UK
SO PCT Int. Appl., 66 pp.
CODEN: PIXXD2
PI WO 9312096 A1 930624
DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 92-GB2334 921216
PRAI GB 91-26677 911216
DT Patent
LA English
IC ICM C07D257-02
ICS C07D255-02; C07D259-00; C07D401-14; C07D409-14
CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
OS MARPAT 120:30786
AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 = (un)substituted alk. chain or heteroatom-contg. chain; Y, Z = **cyclic** polyamine moieties having 9-32 ring members and 3-8 N atoms in the ring spaced by .gtoreq.2 C atoms from each other] or their acid addn. salts or metal complexes are prepd. and demonstrated viricidal activity against **HIV**-1 and **HIV**-2. Thus, 1,1'-[1,4-phenylenebis(methylene)]bis-1,4,8,11-tetraazacyclotetradecane was prepd. and demonstrated 50% inhibitory concn. against **HIV**-1 of 0.006 .mu.g/mL and 50% inhibitory concn. against **HIV**-2 of <0.01 .mu.g/mL in an assay employing infected MT-4 cells.
ST **AIDS** treatment prepn heterocyclic polyamine; **HIV** virucide prepn heterocyclic polyamine; tetraazacyclotetradecane prepn **HIV** viricidal agent; virustat prepn tetraazacyclotetradecane
IT Virucides and Virustats
(heterocyclic polyamines)
IT Virus, animal
(human **immunodeficiency** 1, inhibition of, heterocyclic polyamines for)
IT Virus, animal
(human **immunodeficiency** 2, inhibition of, heterocyclic polyamines for)
IT 151191-32-1 151191-33-2 151191-34-3 151191-35-4 151191-36-5
(**HIV** viricidal activity of)
IT 7440-50-8DP, Copper, 1,4-phenylenebismethylene bis

tetraazacyclotetradecane complexes 7440-66-6DP, Zinc, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes 110078-44-9P 110078-46-1DP, copper and zinc complexes 133587-10-7P 133587-11-8P 151190-72-6P 151190-73-7P 151190-74-8P 151190-75-9P 151190-76-0P 151190-80-6P 151190-81-7P 151190-85-1P 151190-87-3P 151190-91-9P 151190-93-1P 151190-94-2P 151190-95-3P 151190-96-4P 151190-97-5P 151190-98-6P 151190-99-7P 151191-02-5P 151191-03-6P 151191-05-8P 151191-06-9P 151191-08-1P 151191-09-2P 151191-12-7P 151191-14-9P 151191-15-0P 151191-17-2P 151191-18-3P 151191-20-7P 151191-21-8P 151191-24-1P 151191-25-2P 151191-26-3P 151191-27-4P 151191-28-5P 151191-29-6P 151191-30-9P 151191-31-0P 151191-37-6P 151191-38-7P 151191-39-8P
(prepn. and **HIV** viricidal activity of)

IT 19417-58-4P, 1,4-Benzenedipropanol 58791-49-4P 60023-32-7P 63134-93-0P 70364-29-3P 92339-07-6P 105355-16-6P 145617-64-7P 151190-69-1P 151190-70-4P 151190-71-5P 151190-77-1P 151190-79-3P 151190-82-8P 151190-83-9P 151190-84-0P 151190-86-2P 151190-88-4P 151190-89-5P 151190-92-0P 151191-00-3P 151191-01-4P 151191-04-7P 151191-07-0P 151191-10-5P 151191-11-6P 151191-13-8P 151191-16-1P 151191-19-4P 151191-22-9P
(prepn. and reaction of, in prepn. of heterocyclic **HIV** viricidal agents)

IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3, .alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2, Carbethoxymethylene)triphenylphosphorane 1198-37-4, 2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane 7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4 39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1 104395-69-9 110078-46-1 134457-14-0 151190-78-2 151191-23-0
(reaction of, in prepn. of heterocyclic **HIV** viricidal agents)

=> fil reg ;d 151190-77-1
FILE 'REGISTRY' ENTERED AT 13:39:08 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

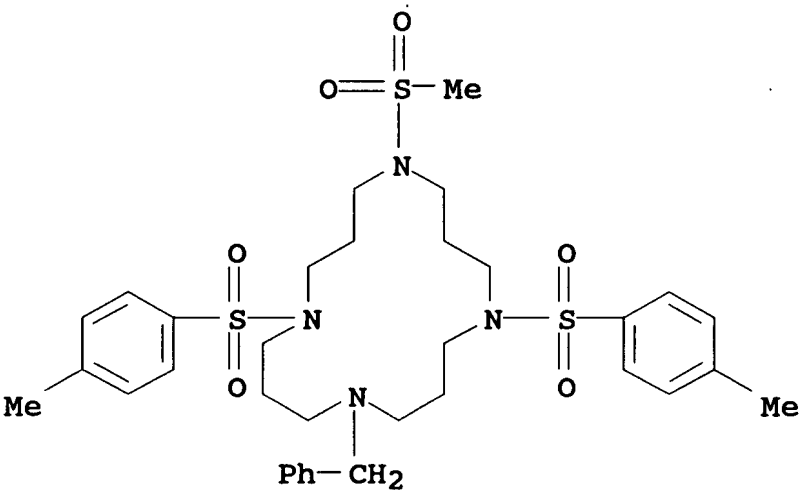
STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when conducting SmartSELECT searches.

ANSWER 1 REGISTRY COPYRIGHT 1995 ACS
RN 151190-77-1 REGISTRY
CN 1,5,9,13-Tetraazacyclohexadecane, 1,9-bis[(4-methylphenyl)sulfonyl]-5-(methylsulfonyl)-13-(phenylmethyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C34 H48 N4 O6 S3

SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

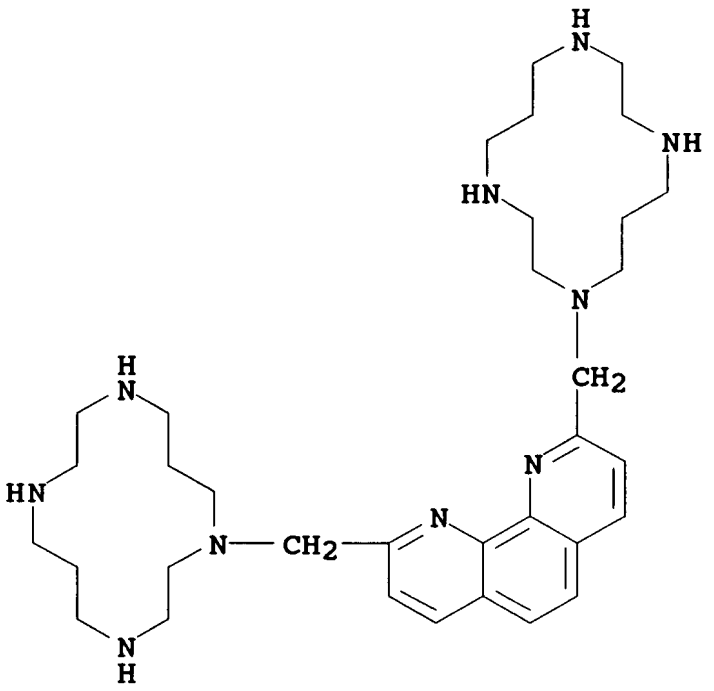
=> fil reg ;d 151190-94-2
FILE 'REGISTRY' ENTERED AT 13:39:35 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when conducting SmartSELECT searches.

ANSWER 1 REGISTRY COPYRIGHT 1995 ACS
RN 151190-94-2 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,10-phenanthroline-2,9-diylbis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C34 H56 N10
CI COM
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

=>
=>

=> fil ca
FILE 'CA' ENTERED AT 13:40:04 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE COVERS 1967 - 18 Mar 1995 (950318/ED) VOL 122 ISS 12

To help control your online searching costs, consider using the HCA File when using the FSEARCH command or when conducting SmartSELECT searches with large numbers of terms.

CAPLUS IS NOW ONLINE!

=>
=> d l10 all

L10 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS
AN 120:30786 CA
TI Linked heterocyclic polyamines with activity against **HIV**
IN **Bridger, Gary James**; Padmanabhan, Sreenivasan; Skerlj, Renato Tony; Thornton, David Michael
PA Johnson Matthey P.L.C., UK
SO PCT Int. Appl., 66 pp.
CODEN: PIXXD2
PI WO 9312096 A1 930624
DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 92-GB2334 921216
PRAI GB 91-26677 911216
DT Patent
LA English
IC ICM C07D257-02
ICS C07D255-02; C07D259-00; C07D401-14; C07D409-14
CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
OS MARPAT 120:30786
AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 = (un)substituted alk. chain or heteroatom-contg. chain; Y, Z = **cyclic** polyamine moieties having 9-32 ring members and 3-8 N atoms in the ring spaced by .gtoreq.2 C atoms from each other] or their acid addn. salts or metal complexes are prepd. and demonstrated viricidal activity against **HIV**-1 and **HIV**-2. Thus, 1,1'-[1,4-phenylenebis(methylene)]bis-1,4,8,11-tetraazacyclotetradecane was prepd. and demonstrated 50% inhibitory concn. against **HIV**-1 of 0.006 .mu.g/mL and 50% inhibitory concn. against **HIV**-2 of <0.01 .mu.g/mL in an assay employing infected MT-4 cells.
ST **AIDS** treatment prepn heterocyclic polyamine; **HIV** virucide prepn heterocyclic polyamine; tetraazacyclotetradecane prepn **HIV** viricidal agent; virustat prepn tetraazacyclotetradecane
IT Virucides and Virustats
(heterocyclic polyamines)
IT Virus, animal
(human **immunodeficiency** 1, inhibition of, heterocyclic polyamines for)

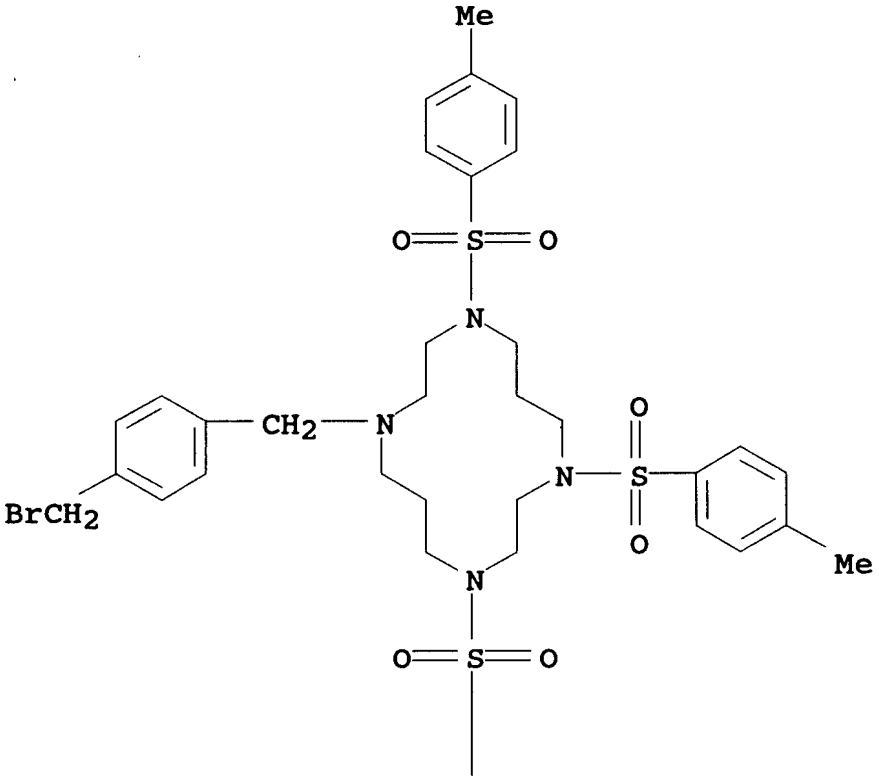
IT Virus, animal
(human **immunodeficiency** 2, inhibition of, heterocyclic polyamines for)
IT 151191-32-1 151191-33-2 151191-34-3 151191-35-4 151191-36-5
(**HIV** viricidal activity of)
IT 7440-50-8DP, Copper, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes 7440-66-6DP, Zinc, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes 110078-44-9P 110078-46-1DP, copper and zinc complexes 133587-10-7P 133587-11-8P 151190-72-6P 151190-73-7P 151190-74-8P 151190-75-9P 151190-76-0P 151190-80-6P 151190-81-7P 151190-85-1P 151190-87-3P 151190-91-9P 151190-93-1P 151190-94-2P 151190-95-3P 151190-96-4P 151190-97-5P 151190-98-6P 151190-99-7P 151191-02-5P 151191-03-6P 151191-05-8P 151191-06-9P 151191-08-1P 151191-09-2P 151191-12-7P 151191-14-9P 151191-15-0P 151191-17-2P 151191-18-3P 151191-20-7P 151191-21-8P 151191-24-1P 151191-25-2P 151191-26-3P 151191-27-4P 151191-28-5P 151191-29-6P 151191-30-9P 151191-31-0P 151191-37-6P 151191-38-7P 151191-39-8P
(prepn. and **HIV** viricidal activity of)
IT 19417-58-4P, 1,4-Benzenedipropanol 58791-49-4P 60023-32-7P 63134-93-0P 70364-29-3P 92339-07-6P 105355-16-6P 145617-64-7P 151190-69-1P 151190-70-4P 151190-71-5P 151190-77-1P 151190-79-3P 151190-82-8P 151190-83-9P 151190-84-0P 151190-86-2P 151190-88-4P 151190-89-5P 151190-92-0P 151191-00-3P 151191-01-4P 151191-04-7P 151191-07-0P 151191-10-5P 151191-11-6P 151191-13-8P 151191-16-1P 151191-19-4P 151191-22-9P
(prepn. and reaction of, in prepn. of heterocyclic **HIV** viricidal agents)
IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3, .alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2, Carbethoxymethylene)triphenylphosphorane 1198-37-4, 2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane 7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4 39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1 104395-69-9 110078-46-1 134457-14-0 151190-78-2 151191-23-0
(reaction of, in prepn. of heterocyclic **HIV** viricidal agents)

=> d l10 all 2

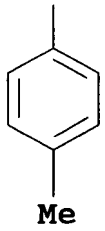
L10 ANSWER 2 OF 2 CA COPYRIGHT 1995 ACS
AN 118:80485 CA
TI Preparation of polyaza(cyclo)alkanes as antiviral compounds
IN Schwartz, David Aaron; **Bridger, Gary**
PA Johnson Matthey PLC, UK
SO PCT Int. Appl., 26 pp.
CODEN: PIXXD2
PI WO 9216494 A1 921001
DS W: AU, CA, FI, HU, JP, KR, NO, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE
AI WO 92-GB438 920311
PRAI GB 91-5489 910315
DT Patent
LA English
IC ICM C07C211-14
ICS C07D257-02; A61K031-13; A61K031-395
CC 23-4 (Aliphatic Compounds)
Section cross-reference(s): 28
OS MARPAT 118:80485
AB Title compds. Z(A)nY (Z, Y = 9 to 32-membered poly(hetero)alkyl chain, -poly(hetero)cycloalkyl moiety, each Z, Y having 3-8 heteroatoms selected from N, O, S such that at least 1 of Z, Y is the above chain; A = linking atom or group; n = 0-6), their salts metal complexes, are prepd. against **HIV** in std. tests. H2N(CH2)CO2H was xl-tosylated, the product esterified with N-hydroxysuccinimide, the ester treated with 1,2,3,4-meso-tetraaminobutane, the tetraamido-tetratosylate treated with borane. THF complex and the product in HBR/AcOH was heated at 100.degree. for 48 h to give meso-1,2,3,4-tetrakis(N-1,3-diaminopropyl)butane (I). In a std. in vitro test I against both **HIV**-1 and **HIV**-1 had a selectivity index (ratio of CD50 and ED50) of >13 compared with AZT >125.
ST tetrakisdiaminopropylbutate prepn virucide **HIV**; tetraazacyclotetradecylbenzomethyl bis prepn virucide **HIV**
IT Virus, animal
(human **immunodeficiency** 1, infection with, treatment of, tetrakis(diaminopropyl)butane and tetraazacyclotetradecylbenzenemethylbis for)
IT Virus, animal
(human **immunodeficiency** 2, infection with, treatment of, tetrakis(diaminopropyl)butane and tetraazacyclotetradecylbenzenemethylbis for)
IT 42908-33-8P 145617-61-4P 145617-62-5P 145617-63-6P 145617-64-7P 145617-65-8P 145617-66-9P 145617-67-0P 145617-68-1P 145617-69-2P
(prepn. and reaction of, in prepn. of **HIV** virucides)
IT 145617-56-7P 145617-57-8P 145617-58-9P 145617-59-0P 145617-60-3P
(prepn. of, as **HIV** virucide)
IT 107-95-9, 3-Aminopropanoic acid 112-24-3 623-24-5 10563-26-5, N,N'-Bis(3-aminopropyl)ethylenediamine 74676-47-4 92902-03-9 104395-69-9
(reaction of, in prepn. of **HIV** virucides)

```
=>
=> fil reg;d 145617-64-7
FILE 'REGISTRY' ENTERED AT 13:40:40 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1995 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:  24 MAR 95   HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95   HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.


ANSWER 1  REGISTRY  COPYRIGHT 1995 ACS
RN   145617-64-7  REGISTRY
CN   1,4,8,11-Tetraazacyclotetradecane, 1-[[4-(bromomethyl)phenyl]methyl]-
     4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI)  (CA INDEX NAME)
FS   3D CONCORD
MF   C39 H49 Br N4 O6 S3
SR   CA
LC   STN Files:   CA
```

PAGE 1-A



PAGE 2-A



2 REFERENCES IN FILE CA (1967 TO DATE)

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 14:07:02 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1995 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:  24 MAR 95   HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95   HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

=>
=> d que l28
L11              STR

N 1       N 3       N 5


NODE ATTRIBUTES:
NSPEC    IS R       AT   1
NSPEC    IS R       AT   3
NSPEC    IS R       AT   5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L13              STR

N— C— Cy— C— N
1   2   3   4   5


NODE ATTRIBUTES:
NSPEC    IS R       AT   1
NSPEC    IS R       AT   5
DEFAULT MLEVEL IS ATOM
GGCAT    IS UNS  AT   3
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   5

STEREO ATTRIBUTES: NONE
L17              STR

Hy— C— Cy— C— Hy
 1   2   3   4   5


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT    IS HIQ  AT   1
```

```
GGCAT   IS UNS  AT   3
GGCAT   IS HIQ  AT   5
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M4 C  M3 N  AT   1
ECOUNT  IS M4 C  M3 N  AT   5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   5

STEREO ATTRIBUTES: NONE
L19             STR
```


```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L22             SCR 1840 AND 1996 AND 140 AND 1607 AND 1236
L23             SCR 1840 AND 1996 AND 140 AND 1607 AND 1363
L28          308 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L17 AND L19 AND
                 (L22 OR L23)

=> fil ca
FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1995 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1967 - 18 Mar 1995 (950318/ED)  VOL 122 ISS 12

  To help control your online searching costs, consider using the
  HCA File when using the FSEARCH command or when conducting
  SmartSELECT searches with large numbers of terms.

CAPLUS IS NOW ONLINE!

=> d his l28-

     (FILE 'REGISTRY' ENTERED AT 13:40:40 ON 25 MAR 95)
L28          308 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23) FUL

     FILE 'CA' ENTERED AT 14:05:18 ON 25 MAR 95
L29           75 S L28
L30            2 S L29(L)(VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IMMU
L31            2 S L29 AND (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IM

     FILE 'REGISTRY' ENTERED AT 14:07:02 ON 25 MAR 95

     FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95
```

=> d all

L31 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS
AN 120:289504 CA
TI Highly potent and selective inhibition of human **immunodeficiency virus** by the bicyclam derivative JM3100
AU De Clerco, Erik; Yamamoto, Naohiko; Pauwels, Rudi; Balzarini, Jan; Witvrouw, Myriam; De Vreese, Karen; Debyser, Zeger; Rosenwirth, Brigitte; Peichl, Peter; et al.
CS Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain, B-3000, Belg.
SO Antimicrob. Agents Chemother. (1994), 38(4), 668-74
CODEN: AMACCQ; ISSN: 0066-4804
DT Journal
LA English
CC 1-5 (Pharmacology)
AB Bicyclams, in which the cyclam (1,4,8,11-tetraazacyclotetradecane) moieties are tethered via an aliph. bridge (i.e., propylene, as in JM2763) are potent and selective inhibitors of human **immunodeficiency virus** type 1 (**HIV**-1) and type-2 (**HIV**-2) (E. De Clercq, N. Yamamoto, R. Pauwels, M. Baba, D. Schols, H. Nakashima, J. Balzarini, Z. Debyser, B. A., Murrer, D. Schwartz, D. Thornton, G. Bridger, S. Fricker, G. Henson, M. Abrams, and D. Picker, Proc. Natl. Acad. Sci. USA 89:5286-5290, 1992). The authors have now found that the bicyclam JM3100, in which the cyclam moieties are tethered by an arom. bridge [i.e., phenylenebis(methylene)], inhibits the replication of various **HIV**-1 and **HIV**-2 strains in various cell lines at a 50% effective concn. (EC50) of 1 to 10 ng/mL, which is about 100-fold lower than the concn. required for JM2763 to inhibit **HIV** replication and at least 100,000-fold lower than the concn. required for JM2763 to inhibit **HIV** replication and at least 100,000-fold lower than the cytotoxic concn. (>500 .mu.g/mL). In primary T4 lymphocytes or primary monocytes, JM3100 proved inhibitory to **HIV**-1 (IIIB) and several clin. **HIV**-1 isolated at an EC50 of less than 1 ng/mL. On the basis of time-of-addn. expts., JM3100 appeared to interact with a viral uncoating event, and this was further corroborated by an uncoating assay in which RNase sensitivity of [5-3H]uridine-labeled virions was monitored. In addn., but possibly mechanistically related, JM3100 blocks formation of infectious particles. JM3100 was also found to interfere directly with **virus**-induced syncytium formation, albeit at a higher concn. (1 to 2 .mu.g/mL) than that required for inhibition of viral replication. Following s.c. injection of 10 mg of JM3100 per kg of body wt. to rabbits, anti-**HIV** activity was detected in serum corresponding to serum drug levels exceeding for at least 6 h by >100-fold the EC50 required to inhibit **HIV** replication in vitro. When combined with either 3'-azido-2',3'-dideoxythymidine or 2',3'-dideoxyinosine, JM3100 achieved a additive inhibition of **HIV** replication, and when repeatedly subcultivated in the presence of JM3100, the **virus** remained insensitive to the compd. for at least 30 passages (120 days) in cell culture.
ST **HIV virus** inhibition bicyclam deriv JM3100
IT **Virucides** and **Virustats**
(bicyclam derivs. as, structure in relation to, in human cells)
IT Drug interactions

(of bicyclam deriv. JM3100 and dideoxynucleosides, in **HIV virus** inhibition in human cells)
IT Drug resistance
(to bicyclam deriv. JM3100, in **HIV virus** in human cells)
IT **Virus**, animal
(human **immunodeficiency** 1, inhibition of, by bicyclam deriv. JM3100, in human cells)
IT **Virus**, animal
(human **immunodeficiency** 2, inhibition of, by bicyclam deriv. JM3100, in human cells)
IT Microbicidal and microbiostatic action
(**virucidal**, of bicyclam deriv. JM3100, against **HIV virus** in human cells)
IT Molecular structure-biological activity relationship
(**virucidal**, of bicyclam derivs., against **HIV virus** in human cells)
IT 30516-87-1, 3'-Azido-2',3'-dideoxythymidine 69655-05-6, 2',3'-Dideoxyinosine
(**HIV virus** inhibition by, bicyclam deriv. JM3100 enhancement of, in human cells)
IT **155148-31-5**
(**HIV virus** inhibition by, mechanism of, structure in relation to, in human cells)
IT 110078-40-5, JM2763 **110078-44-9 151191-06-9 151191-09-2 155148-32-6**
(**HIV virus** inhibition by, structure in relation to, in human cells)

=> fil reg
FILE 'REGISTRY' ENTERED AT 14:07:31 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

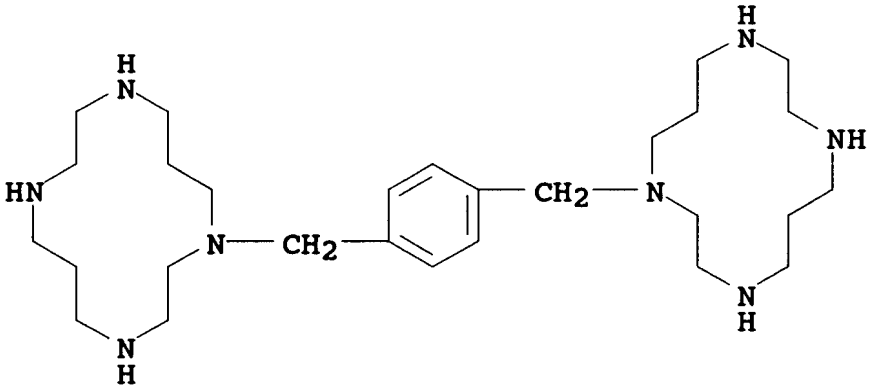
STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when conducting SmartSELECT searches.

=> d 155148-31-5 110078-44-9

ANSWER 1 REGISTRY COPYRIGHT 1995 ACS
RN 155148-31-5 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)
MF C28 H54 N8 . 8 Cl H
SR CA
LC STN Files: CA, TOXLIT
CRN (110078-46-1)

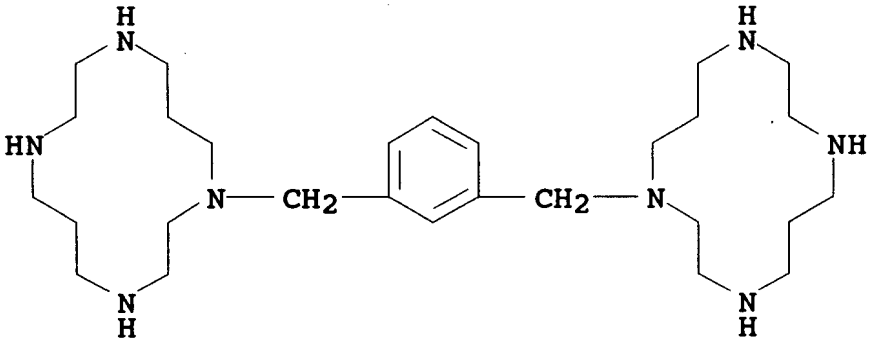


These cmpds are in above

● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 2 REGISTRY COPYRIGHT 1995 ACS
RN 110078-44-9 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8
SR CA
LC STN Files: BEILSTEIN*, CA, CHEMINFORMRX, CJACS, TOXLIT, USPATFULL
(*File contains numerically searchable property data)



5 REFERENCES IN FILE CA (1967 TO DATE)

=>
=>
=>

```
=> fil ca
FILE 'CA' ENTERED AT 14:08:05 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1995 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1967 - 18 Mar 1995 (950318/ED)  VOL 122 ISS 12

  To help control your online searching costs, consider using the
  HCA File when using the FSEARCH command or when conducting
  SmartSELECT searches with large numbers of terms.

CAPLUS IS NOW ONLINE!

=>
=>
=> d all 2

L31  ANSWER 2 OF 2  CA  COPYRIGHT 1995 ACS
AN   120:30786  CA
TI   Linked heterocyclic polyamines with activity against HIV
IN   Bridger, Gary James; Padmanabhan, Sreenivasan; Skerlj, Renato Tony;
     Thornton, David Michael
PA   Johnson Matthey P.L.C., UK
SO   PCT Int. Appl., 66 pp.
     CODEN: PIXXD2
PI   WO 9312096 A1  930624
DS   W:  AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US
     RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI   WO 92-GB2334  921216
PRAI GB 91-26677  911216
DT   Patent
LA   English
IC   ICM  C07D257-02
     ICS  C07D255-02; C07D259-00; C07D401-14; C07D409-14
CC   28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 1
OS   MARPAT 120:30786
AB   The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 =
     (un)substituted alk. chain or heteroatom-contg. chain; Y, Z = cyclic
     polyamine moieties having 9-32 ring members and 3-8 N atoms in the
     ring spaced by .gtoreq.2 C atoms from each other] or their acid
     addn. salts or metal complexes are prepd. and demonstrated viricidal
     activity against HIV-1 and HIV-2.  Thus,
     1,1'-[1,4-phenylenebis(methylene)]bis-1,4,8,11-
     tetraazacyclotetradecane was prepd. and demonstrated 50% inhibitory
     concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory
     concn. against HIV-2 of <0.01 .mu.g/mL in an assay
     employing infected MT-4 cells.
ST   AIDS treatment prepn heterocyclic polyamine; HIV
   virucide prepn heterocyclic polyamine;
     tetraazacyclotetradecane prepn HIV viricidal agent;
   virustat prepn tetraazacyclotetradecane
IT   Virucides and Virustats
        (heterocyclic polyamines)
IT   Virus, animal
        (human immunodeficiency 1, inhibition of, heterocyclic
```

polyamines for)
IT **Virus**, animal
(human **immunodeficiency** 2, inhibition of, heterocyclic polyamines for)
IT **151191-32-1 151191-33-2 151191-34-3**
151191-35-4 151191-36-5
(**HIV** viricidal activity of)
IT 7440-50-8DP, Copper, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes 7440-66-6DP, Zinc, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes
110078-44-9P 110078-46-1DP, copper and zinc complexes **133587-10-7P 133587-11-8P**
151190-72-6P 151190-73-7P 151190-74-8P
151190-75-9P 151190-76-0P 151190-80-6P
151190-81-7P 151190-85-1P **151190-87-3P**
151190-91-9P **151190-93-1P 151190-94-2P**
151190-95-3P 151190-96-4P **151190-97-5P**
151190-98-6P 151190-99-7P 151191-02-5P
151191-03-6P 151191-05-8P 151191-06-9P
151191-08-1P 151191-09-2P 151191-12-7P
151191-14-9P 151191-15-0P **151191-17-2P**
151191-18-3P 151191-20-7P 151191-21-8P
151191-24-1P 151191-25-2P 151191-26-3P
151191-27-4P 151191-28-5P 151191-29-6P
151191-30-9P 151191-31-0P 151191-37-6P
151191-38-7P **151191-39-8P**
(prepn. and **HIV** viricidal activity of)
IT 19417-58-4P, 1,4-Benzenedipropanol 58791-49-4P 60023-32-7P 63134-93-0P 70364-29-3P 92339-07-6P **105355-16-6P** 145617-64-7P 151190-69-1P **151190-70-4P**
151190-71-5P 151190-77-1P 151190-79-3P 151190-82-8P
151190-83-9P 151190-84-0P **151190-86-2P** 151190-88-4P
151190-89-5P **151190-92-0P** 151191-00-3P
151191-01-4P 151191-04-7P 151191-07-0P
151191-10-5P 151191-11-6P 151191-13-8P
151191-16-1P 151191-19-4P 151191-22-9P
(prepn. and reaction of, in prepn. of heterocyclic **HIV** viricidal agents)
IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3, .alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2, Carbethoxymethylene)triphenylphosphorane 1198-37-4, 2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane 7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4 39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1 104395-69-9 **110078-46-1** 134457-14-0 151190-78-2 151191-23-0
(reaction of, in prepn. of heterocyclic **HIV** viricidal agents)

=> d 155148-31-5 110078-46-1 151191-07-0
'155148-31-5' IS NOT A VALID FORMAT FOR FILE 'CA'
'110078-46-1' IS NOT A VALID FORMAT FOR FILE 'CA'
'151191-07-0' IS NOT A VALID FORMAT FOR FILE 'CA'
ENTER DISPLAY FORMAT (BIB):end

=> fil reg

FILE 'REGISTRY' ENTERED AT 14:08:57 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

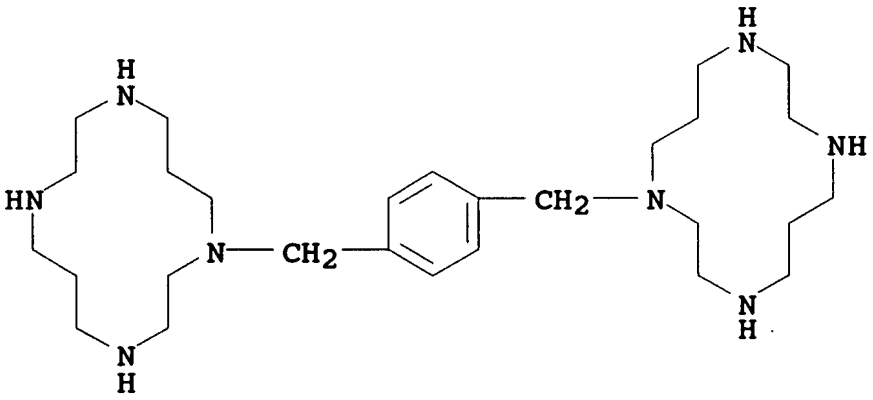
TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when conducting SmartSELECT searches.

=> d 155148-31-5 110078-46-1 151191-07-0

ANSWER 1 REGISTRY COPYRIGHT 1995 ACS
RN 155148-31-5 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)
MF C28 H54 N8 . 8 Cl H
SR CA
LC STN Files: CA, TOXLIT
CRN (110078-46-1)

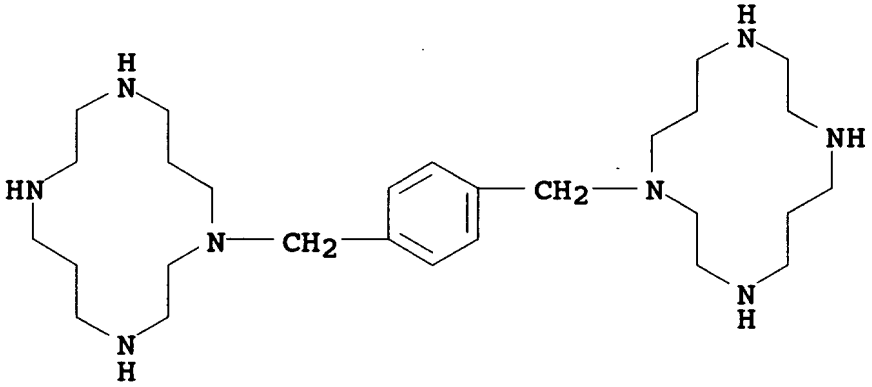
These cmpds are in above



● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

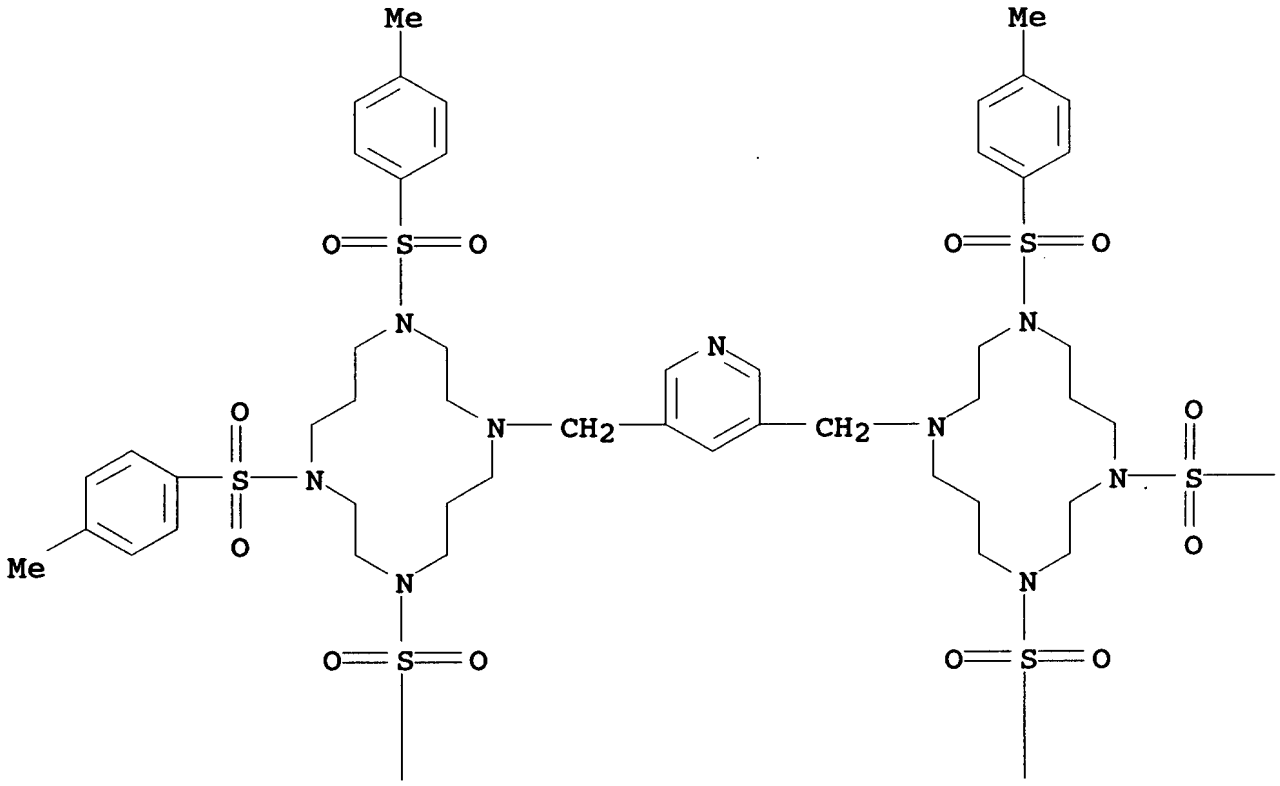
ANSWER 2 REGISTRY COPYRIGHT 1995 ACS
RN 110078-46-1 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8
CI COM
SR CA
LC STN Files: BEILSTEIN*, CA, CJACS, USPATFULL
(*File contains numerically searchable property data)



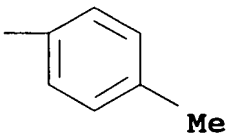
4 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

ANSWER 3 REGISTRY COPYRIGHT 1995 ACS
RN 151191-07-0 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediylbis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C69 H89 N9 O12 S6
SR CA
LC STN Files: CA

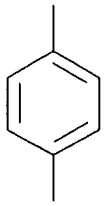
PAGE 1-A

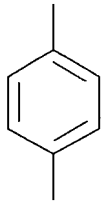


PAGE 1-B



PAGE 2-A





1 REFERENCES IN FILE CA (1967 TO DATE)

=> d his

(FILE 'HOME' ENTERED AT 13:27:42 ON 25 MAR 95)

FILE 'REGISTRY' ENTERED AT 13:28:34 ON 25 MAR 95

L1 STR
L2 SCR 1847 AND 1996
L3 50 S L1 AND L2
L4 STR
L5 17 S L1 AND L4
L6 50 S L1 AND L4 AND L2

FILE 'CA' ENTERED AT 13:36:51 ON 25 MAR 95

L7 37 S BRIDGER G?/AU
L8 2 S L7 AND (HIV OR AIDS OR HTLV OR IMMUNODEFIC?)
L9 1 S L7 AND CYCLIC
L10 2 S L8 OR L9

FILE 'REGISTRY' ENTERED AT 13:39:08 ON 25 MAR 95

```
     FILE 'REGISTRY' ENTERED AT 13:39:35 ON 25 MAR 95

     FILE 'CA' ENTERED AT 13:40:04 ON 25 MAR 95

     FILE 'REGISTRY' ENTERED AT 13:40:40 ON 25 MAR 95
L11             STR L1
L12             STR L4
L13             STR L12
L14           0 S L11 AND L12 AND L13
L15             SCR 1840 AND 1996
L16           4 S L11 AND L12 AND L13 AND L15
L17             STR L12
L18           3 S L11 AND L13 AND L17 AND L15
L19             STR
L20           4 S L11 AND L13 AND L17 AND L19 AND L15
L21           7 S L11 AND L13 AND L19 AND L15
L22             SCR 1840 AND 1996 AND 140 AND 1607 AND 1236
L23             SCR 1840 AND 1996 AND 140 AND 1607 AND 1363
L24          14 S L11 AND L13 AND L19 AND (L22 OR L23)
L25           8 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23)
L26          50 S L1 AND L13 AND L17 AND L19 AND (L22 OR L23)
L27          50 S L25 OR L26
L28         308 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23) FUL

     FILE 'CA' ENTERED AT 14:05:18 ON 25 MAR 95
L29          75 S L28
L30           2 S L29(L)(VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IMMU
L31           2 S L29 AND (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IM

     FILE 'REGISTRY' ENTERED AT 14:07:02 ON 25 MAR 95

     FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95

     FILE 'REGISTRY' ENTERED AT 14:07:31 ON 25 MAR 95

     FILE 'CA' ENTERED AT 14:08:05 ON 25 MAR 95

     FILE 'REGISTRY' ENTERED AT 14:08:57 ON 25 MAR 95

     FILE 'CA' ENTERED AT 14:09:21 ON 25 MAR 95
L32           4 S L29 AND PHARMAC?/SC,SX
L33           2 S L32 NOT L31

=>
=>
=> d all

L33  ANSWER 1 OF 2  CA  COPYRIGHT 1995 ACS
AN   118:160633  CA
TI   Synthesis, DNA binding interactions and biological activity of
     bis-platinum (II) complexes of N,N,N',N'-tetrakis(2-
     aminoethyl)diamines
AU   Palmer, Brian D.; Wickham, Geoffrey; Craik, David J.; McFadyen, W.
     David; Wakelin, Laurence P. G.; Baguley, Bruce C.; Denny, William A.
CS   Sch. Med., Univ. Auckland, Auckland, N. Z.
SO   Anti-Cancer Drug Des. (1992), 7(5), 385-401
```

CODEN: ACDDEA; ISSN: 0266-9536
DT Journal
LA English
CC 1-6 (**Pharmacology**)
Section cross-reference(s): 23, 25, 78
AB A series of dimers of the monofunctional platinum species [Pt(dien)Cl]+, linked by a variety of flexible (polymethylene) and more rigid chains, was prepd. and evaluated for DNA interactions and cytotoxic activity. The polymethylene-linked dimers were prepd. by acylation of N1,N3-bistrityldiethylenetriamine with .alpha.,.omega.-dicarboxylic acid chlorides, followed by redn. with diborane. Platination of these ligands was achieved with K2PtI4 prepd. in situ, followed by anion exchange. Solns. of the bis(Pt(dien)Cl)2+ complexes were stable, and shown to be pure by 195Pt NMR, but solid products could not be isolated. All of the bis(Pt(dien)Cl)2+ complexes unwound closed circular supercoiled DNA more efficiently than the monomer, and were more efficient than the difunctional platinum complex cisplatin at crosslinking linearized plasmid NDA, as measured on non-denaturing agarose gels. None of the bis(Pt(dien)Cl)2+ complexes were as cytotoxic as cisplatin in both the wild-type and platinum-resistant P388 murine leukemia cell lines. The more rigid analogs were equitoxic in both sensitive and cisplatin-resistant cells, but none showed in vitro activity against the P388 tumor.
ST tetrakisaminoethyldiamine platinum complex antitumor prepn; aminoethyldiamine platinum complex antitumor prepn
IT Deoxyribonucleic acids
(bis-platinum tetrakis(aminoethyl)diamine complexes binding of, antitumor activity in relation to)
IT Neoplasm inhibitors
(bis-platinum tetrakis(aminoethyl)diamine complexes, prepn. and DNA binding of)
IT Crosslinking
(of bis-platinum tetrakis(aminoethyl)diamine complexes, by DNA)
IT Kinetics, reaction
(of platinum tetrakis(aminoethyl)diamine complexes, with DNA, antitumor activity in relation to)
IT 79-37-8, Oxalyl chloride 543-20-4, Succinyl chloride 1663-67-8, Malonyl chloride 90421-57-1
(acylation by, of bistrityldiethylenamine)
IT 100-39-0, Benzyl bromide
(alkylation by, of bistrityldiethylenamine)
IT 623-24-5 626-15-3 628-77-3, 1,5-Diiodopentane
(alkylation by, of bistrityldiethylenetriamine)
IT 76-83-5, Trityl chloride
(alkylation by, of diethylenetriamine)
IT 15663-27-1
(antitumor activity and DNA binding interaction of, aminoethyldiamine platinum complexes in relation to)
IT 1877-77-6, 3-(Hydroxymethyl)aniline
(chlorine substitution reaction of)
IT 10025-99-7
(complexation of, with diamines)
IT 6232-88-8, 4-(Bromomethyl)benzoic acid
(conversion of, to acid chloride)
IT 145901-58-2P
(prepn. and alkylation of, with benzyl halides or

haloalkylbenzamide derivs.)
IT 876-08-4P, 4-(Chloromethyl)benzoyl chloride
(prepn. and amidation by, of (chloromethyl)aniline)
IT 145883-50-7P
(prepn. and amidation of, with (chloromethyl)benzoyl chloride)
IT 14215-58-8P 18509-61-0P 145901-59-3P 146283-44-5P
146283-45-6P **146283-46-7P** **146283-47-8P**
146283-48-9P **146291-98-7P** 146755-38-6P
(prepn. and antitumor activity of, DNA binding interaction in relation to)
IT 145883-53-0P
(prepn. and complexation with platinum complexes)
IT 146735-46-8P
(prepn. and conversion to chloride complex)
IT 145883-52-9P 145883-54-1P 145883-59-6P
(prepn. and detritylation of)
IT 145883-51-8P
(prepn. and reaction with bistrityldiethylenetriamine)
IT 23539-10-8P 71277-15-1P 73571-38-7P 142745-41-3P
145883-55-2P 145883-61-0P 145883-62-1P
(prepn. and reaction with platinum complexes)
IT 145883-58-5P
(prepn. and redn. of)
IT 13528-04-6P 145883-56-3P 145883-57-4P 145883-60-9P
(prepn. of)
IT 111-40-0, Diethylenetriamine
(tritylation of)

These cmpds are in above

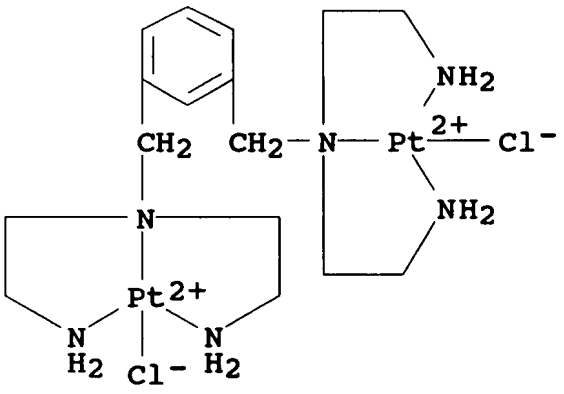
=> fil reg;d 146283-46-7 146283-47-8 146291-98-7
FILE 'REGISTRY' ENTERED AT 14:10:36 ON 25 MAR 95

STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when conducting SmartSELECT searches.

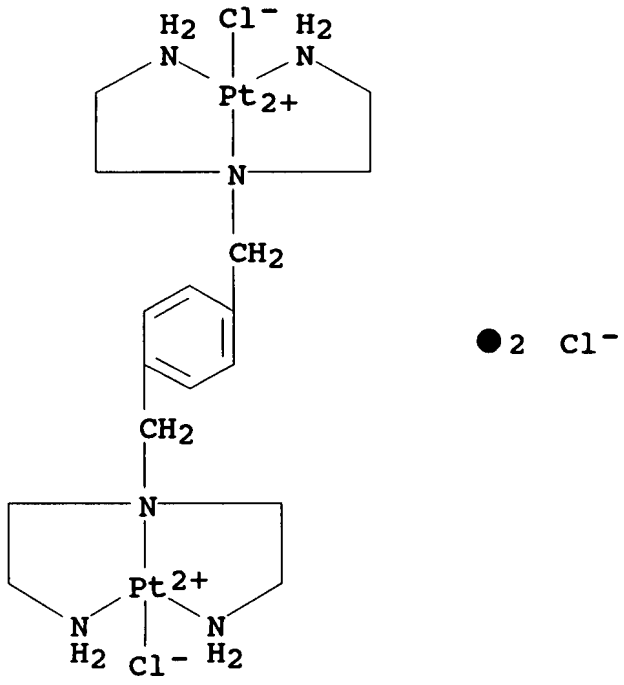
ANSWER 1 REGISTRY COPYRIGHT 1995 ACS
RN 146283-46-7 REGISTRY
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1,3-benzenedimethanamine-N1,N1',N1'':N3,N3',N3'']]di-, dichloride (9CI) (CA INDEX NAME)
MF C16 H32 Cl2 N6 Pt2 . 2 Cl
CI CCS
SR CA
LC STN Files: CA, TOXLIT



● 2 Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)

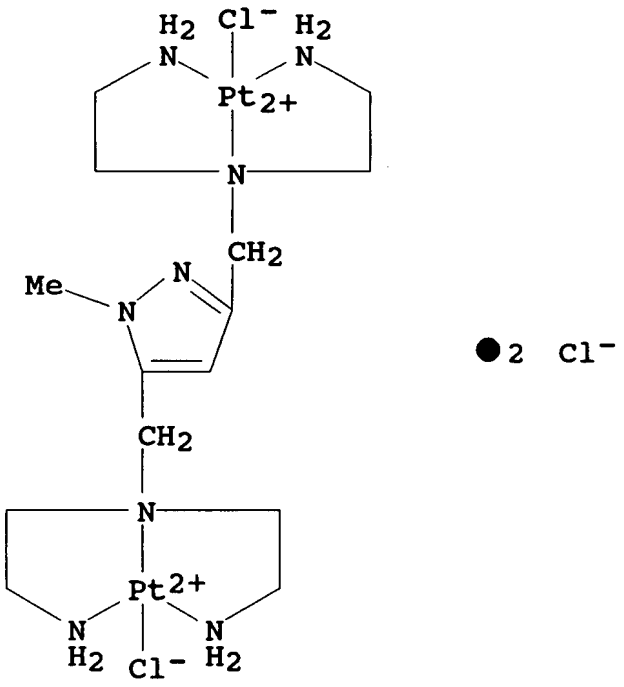
ANSWER 2 REGISTRY COPYRIGHT 1995 ACS
RN 146283-47-8 REGISTRY
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1,4-benzenedimethanamine-N1,N1',N1'':N4,N4',N4'']]di-, dichloride (9CI) (CA INDEX NAME)
MF C16 H32 Cl2 N6 Pt2 . 2 Cl
CI CCS
SR CA
LC STN Files: CA, TOXLIT



● 2 Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 3 REGISTRY COPYRIGHT 1995 ACS
RN 146291-98-7 REGISTRY
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1-methyl-1H-pyrazole-3,5-dimethanamine-N3,N3',N3'':N5,N5',N5'']]di-, dichloride (9CI) (CA INDEX NAME)
MF C14 H32 Cl2 N8 Pt2 . 2 Cl
CI CCS
SR CA
LC STN Files: CA, TOXLIT



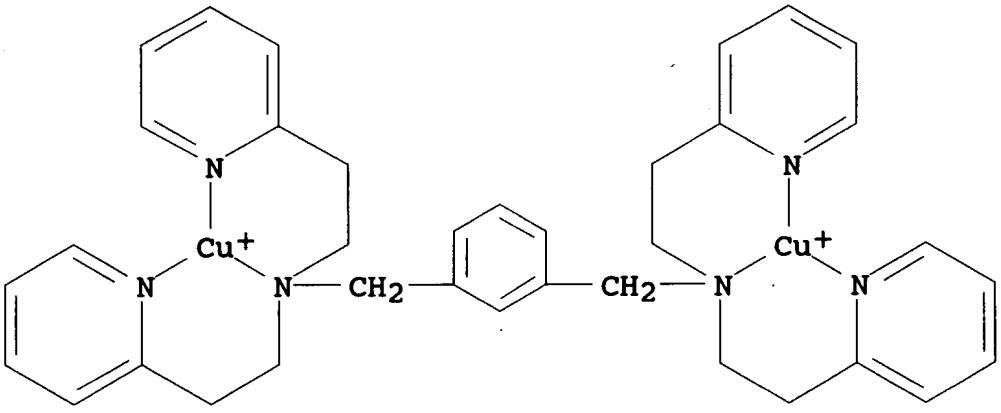
●2 Cl-

1 REFERENCES IN FILE CA (1967 TO DATE)

```
=> fil ca
FILE 'CA' ENTERED AT 14:10:51 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1995 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1967 - 18 Mar 1995 (950318/ED)  VOL 122 ISS 12

  To help control your online searching costs, consider using the
  HCA File when using the FSEARCH command or when conducting
  SmartSELECT searches with large numbers of terms.

CAPLUS IS NOW ONLINE!

=>
=> d all  2

L33  ANSWER 2 OF 2  CA  COPYRIGHT 1995 ACS
AN   97:119531  CA
TI   Three-coordinate binuclear copper(I) complex:  model compound for
     the copper sites in deoxyhemocyanin and deoxytyrosinase
AU   Karlin, Kenneth D.; Gultneh, Yilma; Hutchinson, John P.; Zubieta,
     Jon
CS   Cent. Biol. Macromol., State Univ. New York, Albany, NY, 12222, USA
SO   J. Am. Chem. Soc. (1982), 104(19), 5240-2
     CODEN: JACSAT; ISSN: 0002-7863
DT   Journal
LA   English
CC   78-7 (Inorganic Chemicals and Reactions)
     Section cross-reference(s): 1, 75
OS   CJACS
AB   The deoxy-binuclear Cu contg. active sites in the dioxygen carrier
     hemocyanin and the monooxygenase tyrosinase are through to contain 2
     Cu(I) ions in close proximity which are each 2 or 3 coordinate and
     ligated to nitrogenous ligands.  The synthesis and x-ray structural
     characterization of [Cu2L](PF6)2 (I) (L = 1,3-[(RCH2CH2)2NCH2]2C6H4,
     where = pyridyl) which mimics features of these deoxy sites is
     described.  I contains a binucleating ligand where 2 tridentate
     groups with pyridyl and amino N-donors are connected by a m-xylyl
     connecting group.  Each crystallog. independent Cu(I) ion is
     3-coordinate in a similar distorted trigonal planar geometry with
     bonding parameters (av.); Cu-N(amino) = 2.16 .ANG.; Cu-N(pyridyl) =
     1.92 .ANG.; N(amino)-Cu-N(pyridyl) = 99.8-104.3.degree.
     N(pyridyl)-Cu-N(pyridyl) = 150.9.degree..  The Cu(I) moieties are
     extended away from each other; Cu. . .Cu = 8.940(2) .ANG..  I reacts
     with O in a manner analogous to the monooxygenases; it shows a
     quasireversible oxidn. wave at E1/2 = +0.16 V vs. NHE in DMF and
     reacts with CO and P-contg. ligands.
ST   copper pyridylaminoxylyl complex; crystal structure copper
     pyridylaminoxylyl; xylyl pyridylamino copper complex
IT   Crystal structure
     Molecular structure
        (of copper bis[bis(pyridylethyl)amino]-m-xylyl binuclear complex)
IT 82731-39-3P
        (prepn. and crystal structure of)
IT   64443-05-6
        (reaction of, with bis[bis(pyridylethyl)amino]-m-xylyl)
```

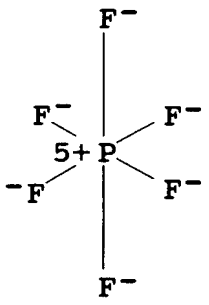
```
=> fil reg ;d 82731-39-3
FILE 'REGISTRY' ENTERED AT 14:11:13 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1995 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:  24 MAR 95   HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95   HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.


ANSWER 1  REGISTRY  COPYRIGHT 1995 ACS
RN   82731-39-3  REGISTRY
CN   Copper(2+), [.mu.-[N,N,N',N'-tetrakis[2-(2-pyridinyl)ethyl]-1,3-
     benzenedimethanamine-N1,N1',N1'':N3,N3',N3'']]di-,
     bis[hexafluorophosphate(1-)] (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   1,3-Benzenedimethanamine, N,N,N',N'-tetrakis[2-(2-pyridinyl)ethyl]-,
     copper complex
CN   Phosphate(1-), hexafluoro-, [.mu.-[N,N,N',N'-tetrakis[2-(2-
     pyridinyl)ethyl]-1,3-benzenedimethanamine-
     N1,N1',N1'':N3,N3',N3'']]dicopper(2+) (2:1)
MF   C36 H40 Cu2 N6 . 2 F6 P
LC   STN Files:   CA, CJACS

     CM   1

     CRN  82281-84-3
     CMF  C36 H40 Cu2 N6
     CCI  CCS
```

These cmpds are in above ste




```
     CM   2

     CRN  16919-18-9
     CMF  F6 P
```

CCI CCS

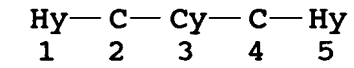


2 REFERENCES IN FILE CA (1967 TO DATE)

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 14:27:59 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 1995 American Chemical Society (ACS)

STRUCTURE FILE UPDATES:  24 MAR 95   HIGHEST RN 161753-30-6
DICTIONARY FILE UPDATES: 24 MAR 95   HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

=> d que l40
L11              STR

N 1       N 3       N 5


NODE ATTRIBUTES:
NSPEC    IS R       AT    1
NSPEC    IS R       AT    3
NSPEC    IS R       AT    5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L13              STR

N— C— Cy— C— N
1   2   3   4   5


NODE ATTRIBUTES:
NSPEC    IS R       AT    1
NSPEC    IS R       AT    5
DEFAULT MLEVEL IS ATOM
GGCAT    IS UNS  AT    3
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   5

STEREO ATTRIBUTES: NONE
L17              STR

Hy— C— Cy— C— Hy
 1   2   3   4   5


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT    IS HIQ  AT    1
GGCAT    IS UNS  AT    3
GGCAT    IS HIQ  AT    5
```

```
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M4 C  M3 N  AT   1
ECOUNT  IS M4 C  M3 N  AT   5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   5

STEREO ATTRIBUTES: NONE
L19             STR
```


```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L22             SCR 1840 AND 1996 AND 140 AND 1607 AND 1236
L23             SCR 1840 AND 1996 AND 140 AND 1607 AND 1363
L28         308 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L17 AND L19 AND
                 (L22 OR L23)
L36             STR
```

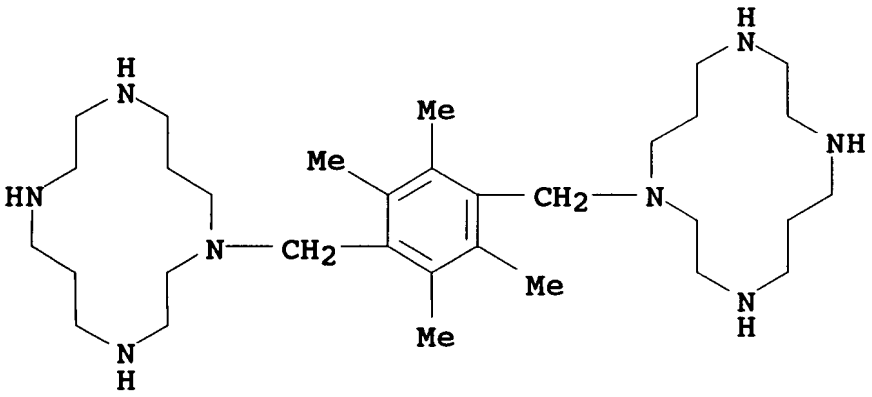



```
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS HIQ  AT   1
GGCAT   IS UNS  AT   3
GGCAT   IS HIQ  AT   5
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M8 C  E4 N  AT   1
ECOUNT  IS M8 C  E4 N  AT   5

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   5

STEREO ATTRIBUTES: NONE
L40         137 SEA FILE=REGISTRY SUB=L28 SSS FUL L36

=> d his l41-

     (FILE 'REGISTRY' ENTERED AT 14:11:13 ON 25 MAR 95)
L41          60 S L38 AND L40
L42             STR
L43          50 S L42
L44      111859 S 591.79.52/RID
L45          50 S L43 NOT L41
L46          57 S L41 NOT L44
```

FILE 'REGISTRY' ENTERED AT 14:27:59 ON 25 MAR 95

=> d 1-7 ide can

L46 ANSWER 1 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 158200-26-1 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,3,5,6-tetramethyl-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H62 N8
SR CA
LC STN Files: CA

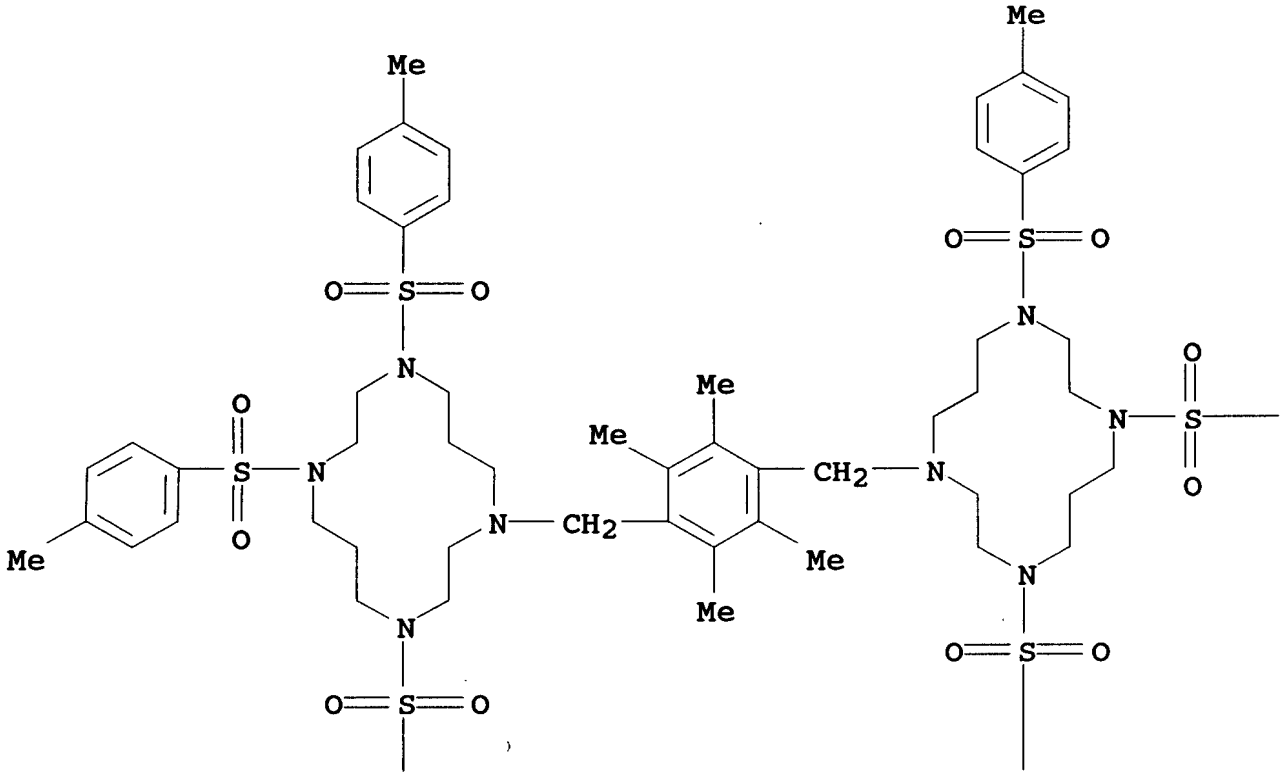


1 REFERENCES IN FILE CA (1967 TO DATE)

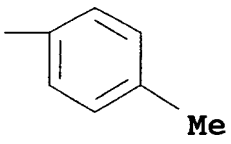
REFERENCE 1: 121:225706

L46 ANSWER 2 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 158200-25-0 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,3,5,6-tetramethyl-1,4-phenylene)bis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C74 H98 N8 O12 S6
SR CA
LC STN Files: CA

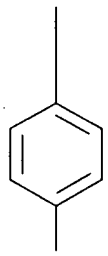
PAGE 1-A

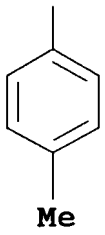


PAGE 1-B



PAGE 2-A

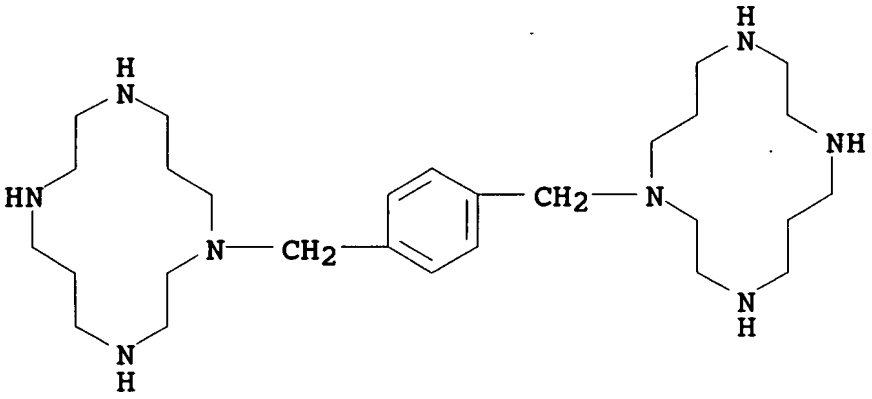




1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 121:225706

L46 ANSWER 3 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 155148-32-6 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrobromide (9CI) (CA INDEX NAME)
MF C28 H54 N8 . 8 Br H
SR CA
LC STN Files: CA, TOXLIT
CRN (110078-46-1)



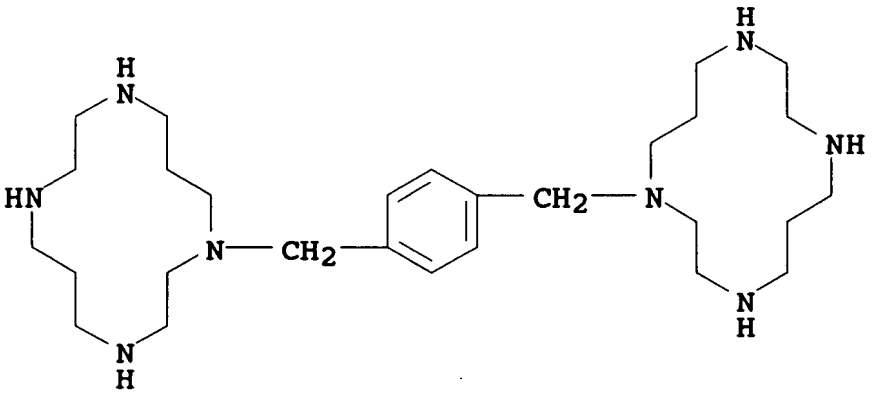
● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

L46 ANSWER 4 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 155148-31-5 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)
MF C28 H54 N8 . 8 Cl H

SR CA
LC STN Files: CA, TOXLIT
CRN (110078-46-1)



●8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

L46 ANSWER 5 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151987-13-2 REGISTRY
CN Cobalt(2+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']]bis[carbonato(2-)-O,O']di-, dichloride, stereoisomer (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,4,7,10-Tetraazacyclododecane, cobalt(2+) deriv. (9CI)
MF C34 H50 Co2 N8 O6 . 2 Cl
CI CCS
SR CA
LC STN Files: CA
DES *

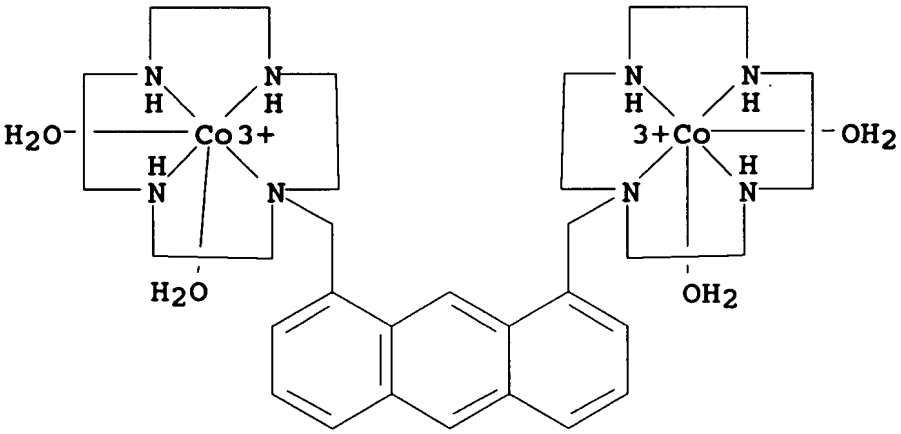
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:44414

L46 ANSWER 6 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151956-64-8 REGISTRY
CN Cobalt(6+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']]tetraaquadi-, stereoisomer, hexanitrate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,4,7,10-Tetraazacyclododecane, cobalt(6+) deriv. (9CI)
MF C32 H58 Co2 N8 O4 . 6 N O3
SR CA
LC STN Files: CA

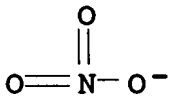
CM 1

CRN 151956-63-7
CMF C32 H58 Co2 N8 O4
CCI CCS
CDES *



CM 2

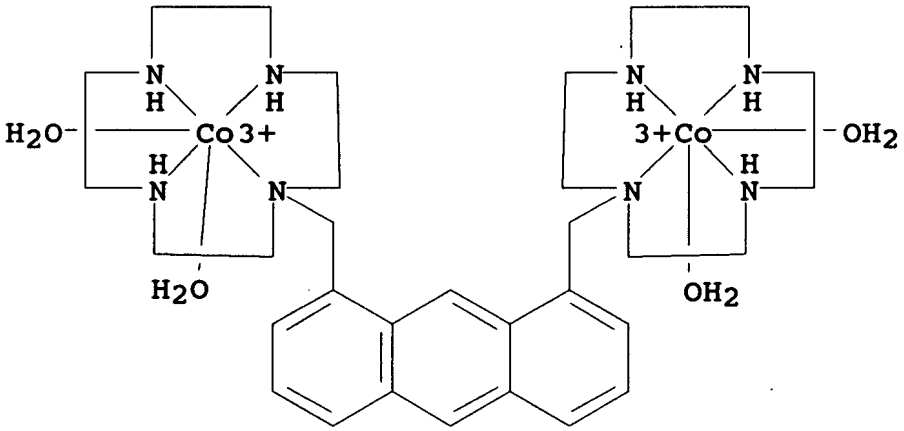
CRN 14797-55-8
CMF N O3



1 REFERENCES IN FILE CA (1967 TO DATE)

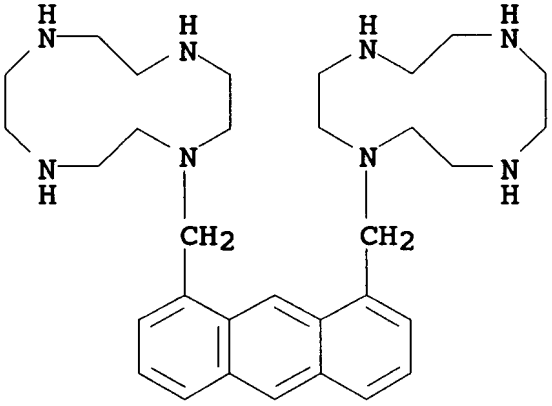
REFERENCE 1: 120:44414

L46 ANSWER 7 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151956-63-7 REGISTRY
CN Cobalt(6+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']]tetraaquadi-, stereoisomer (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,4,7,10-Tetraazacyclododecane, cobalt(6+) deriv. (9CI)
MF C32 H58 Co2 N8 O4
CI CCS, COM
SR CA
DES *



=> d 8-30 ide can

L46 ANSWER 8 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151697-44-8 REGISTRY
CN 1,4,7,10-Tetraazacyclododecane, 1,1'-[1,8-anthracenediylbis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)
MF C32 H50 N8 . 8 Cl H
SR CA
LC STN Files: CA



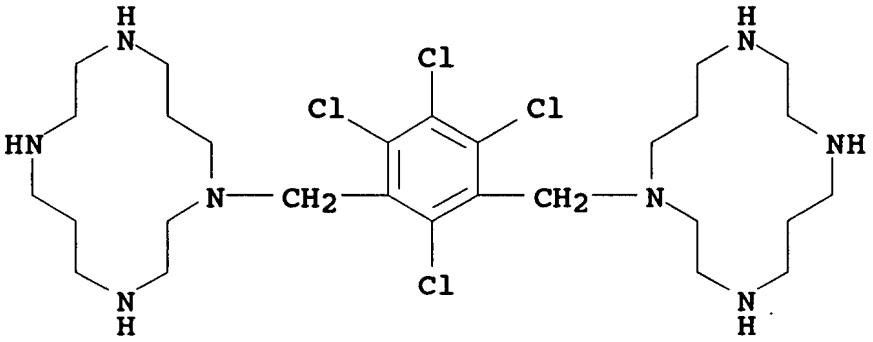
●8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:44414

L46 ANSWER 9 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-34-3 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,4,5,6-tetrachloro-1,3-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)

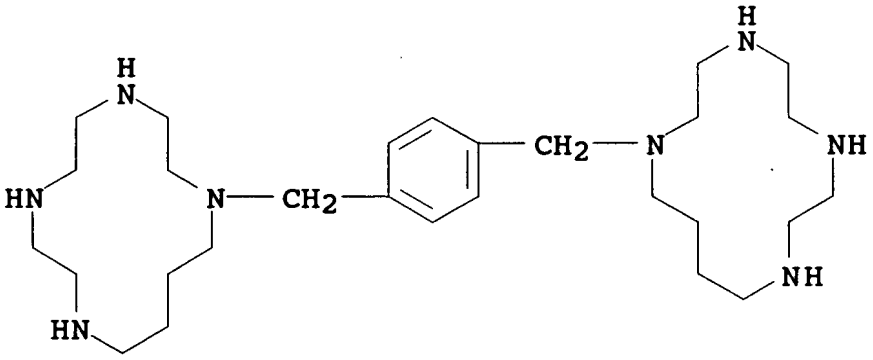
FS 3D CONCORD
MF C28 H50 Cl4 N8
CI COM
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 10 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-33-2 REGISTRY
CN 1,4,7,10-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8
SR CA
LC STN Files: CA

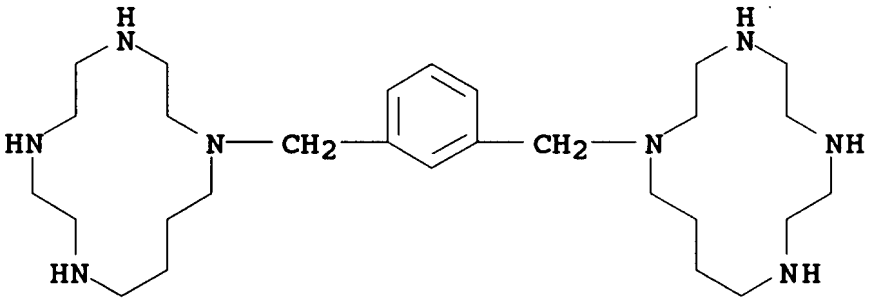


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 11 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-32-1 REGISTRY
CN 1,4,7,10-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8

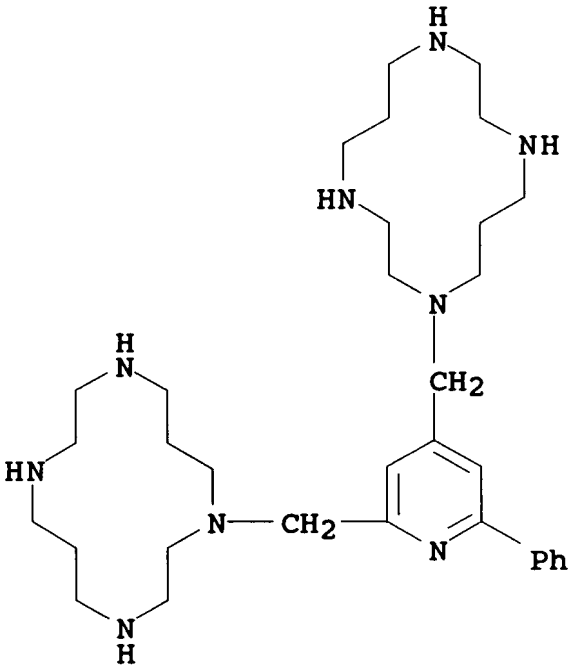
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

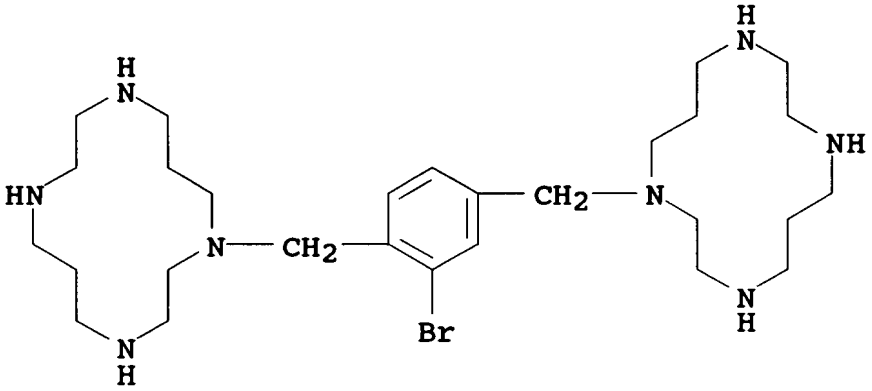
L46 ANSWER 12 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-31-0 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(6-phenyl-2,4-pyridinediyl)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C33 H57 N9
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

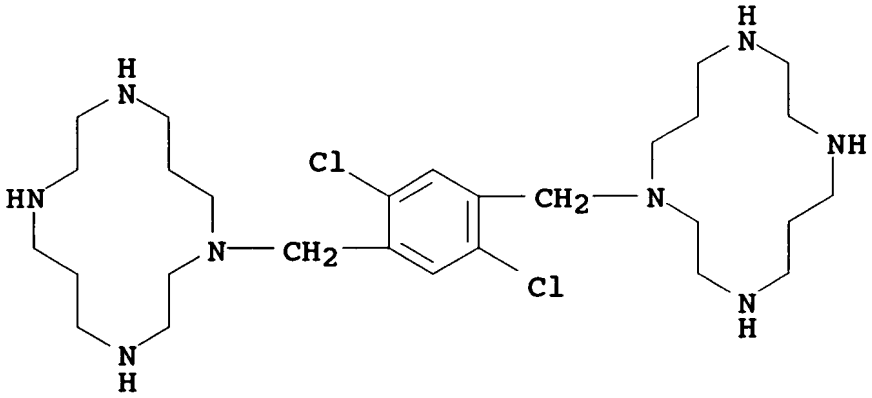
L46 ANSWER 13 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-30-9 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2-bromo-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H53 Br N8
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 14 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-29-6 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,5-dichloro-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H52 Cl2 N8
SR CA
LC STN Files: CA

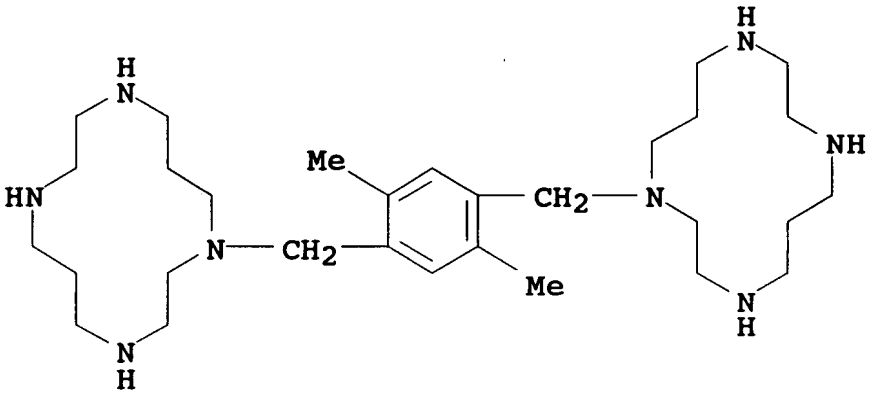


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 15 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-28-5 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,5-dimethyl-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C30 H58 N8
SR CA
LC STN Files: CA

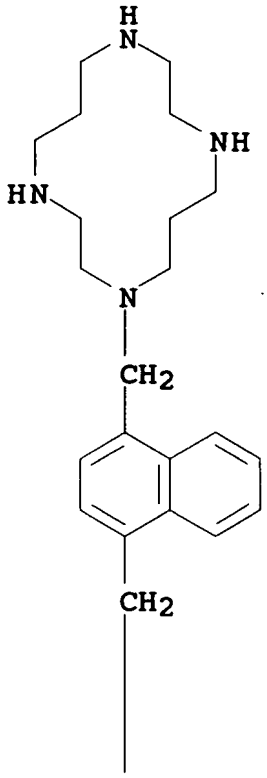


1 REFERENCES IN FILE CA (1967 TO DATE)

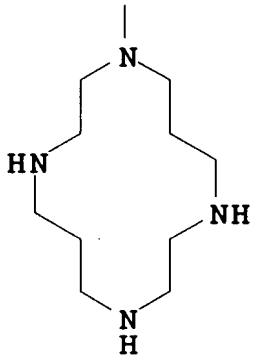
REFERENCE 1: P 120:30786

L46 ANSWER 16 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-27-4 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-naphthalenediylbis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H56 N8
CI COM
SR CA
LC STN Files: CA

PAGE 1-A



PAGE 2-A

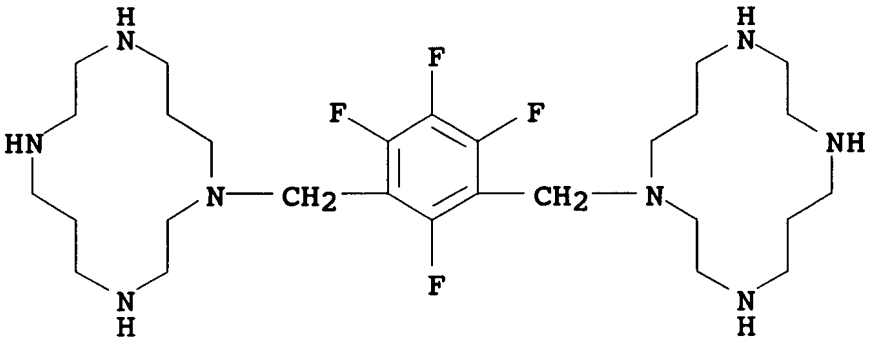


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 17 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-26-3 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[(2,4,5,6-tetrafluoro-1,3-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H50 F4 N8
SR CA

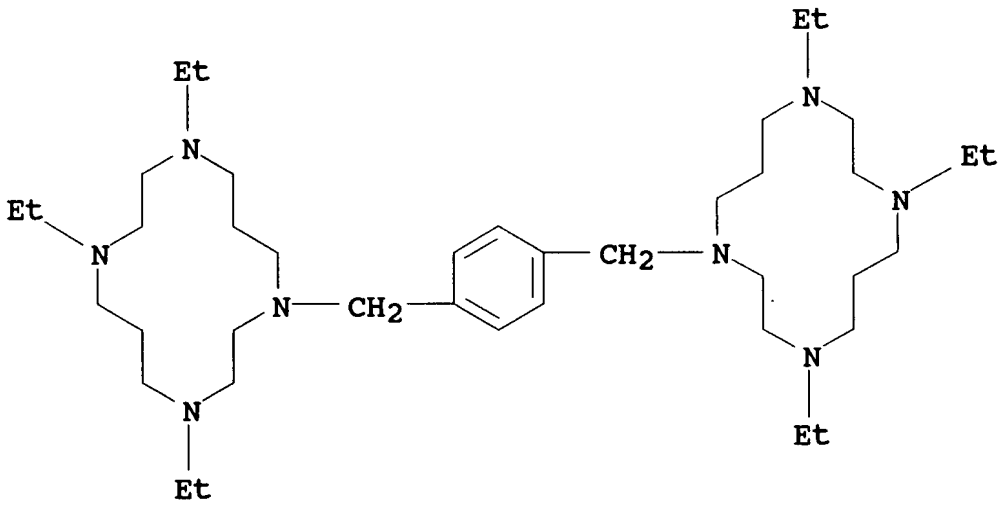
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 18 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-21-8 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C40 H78 N8
CI COM
SR CA
LC STN Files: CA

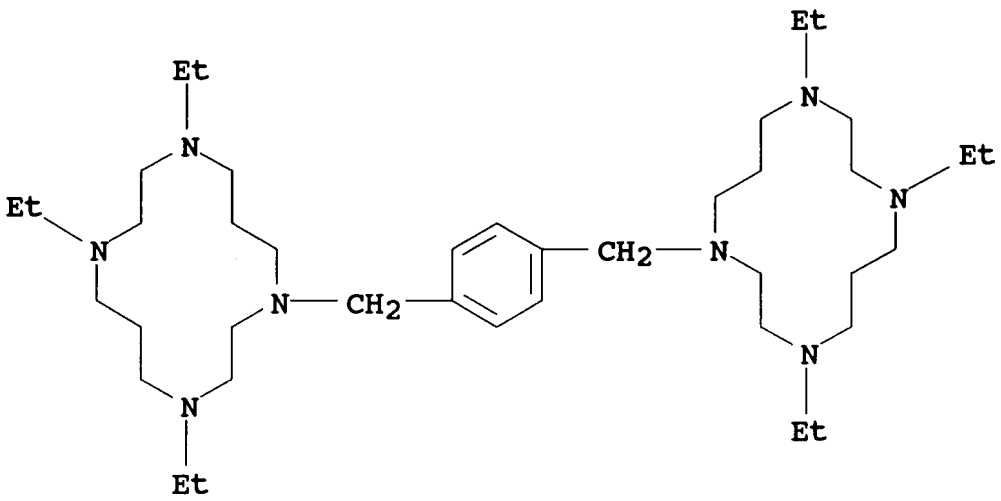


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 19 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-20-7 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triethyl-, octahydrobromide (9CI)

(CA INDEX NAME)
MF C40 H78 N8 . 8 Br H
SR CA
LC STN Files: CA
CRN (151191-21-8)

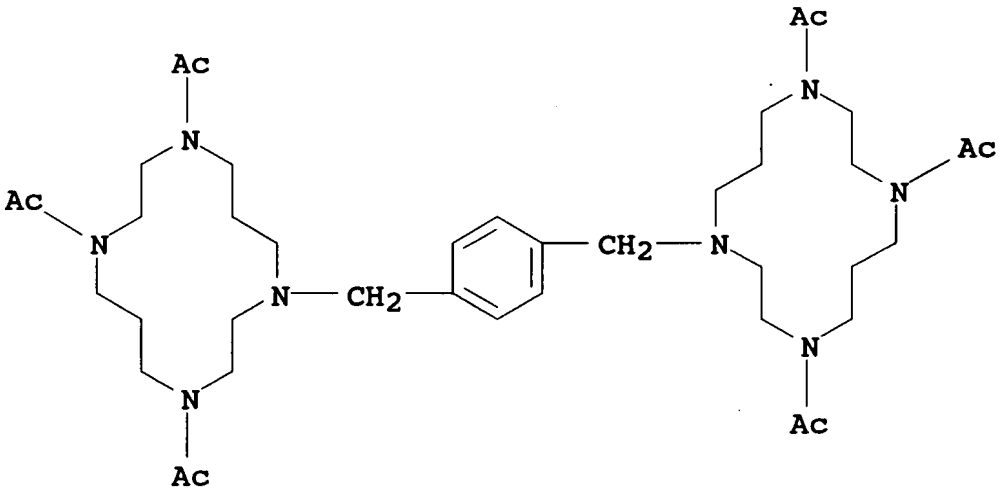


● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

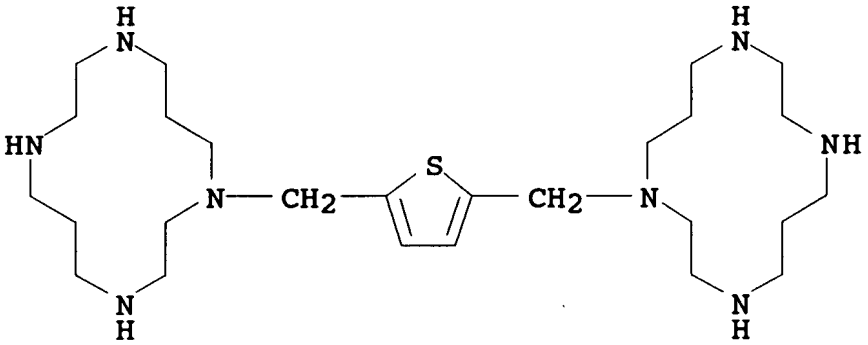
L46 ANSWER 20 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-19-4 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triacetyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C40 H66 N8 O6
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 21 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-18-3 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,5-thiophenediylbis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H52 N8 S
CI COM
SR CA
LC STN Files: CA

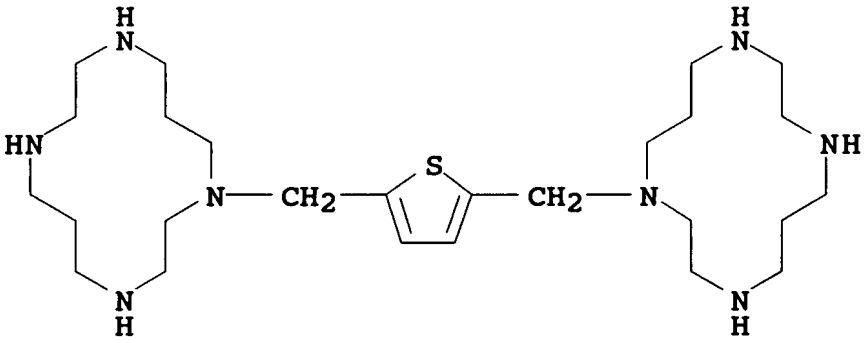


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 22 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-17-2 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,5-thiophenediylbis(methylene)]bis-, octahydrobromide (9CI) (CA INDEX NAME)
MF C26 H52 N8 S . 8 Br H

SR CA
LC STN Files: CA
CRN (151191-18-3)



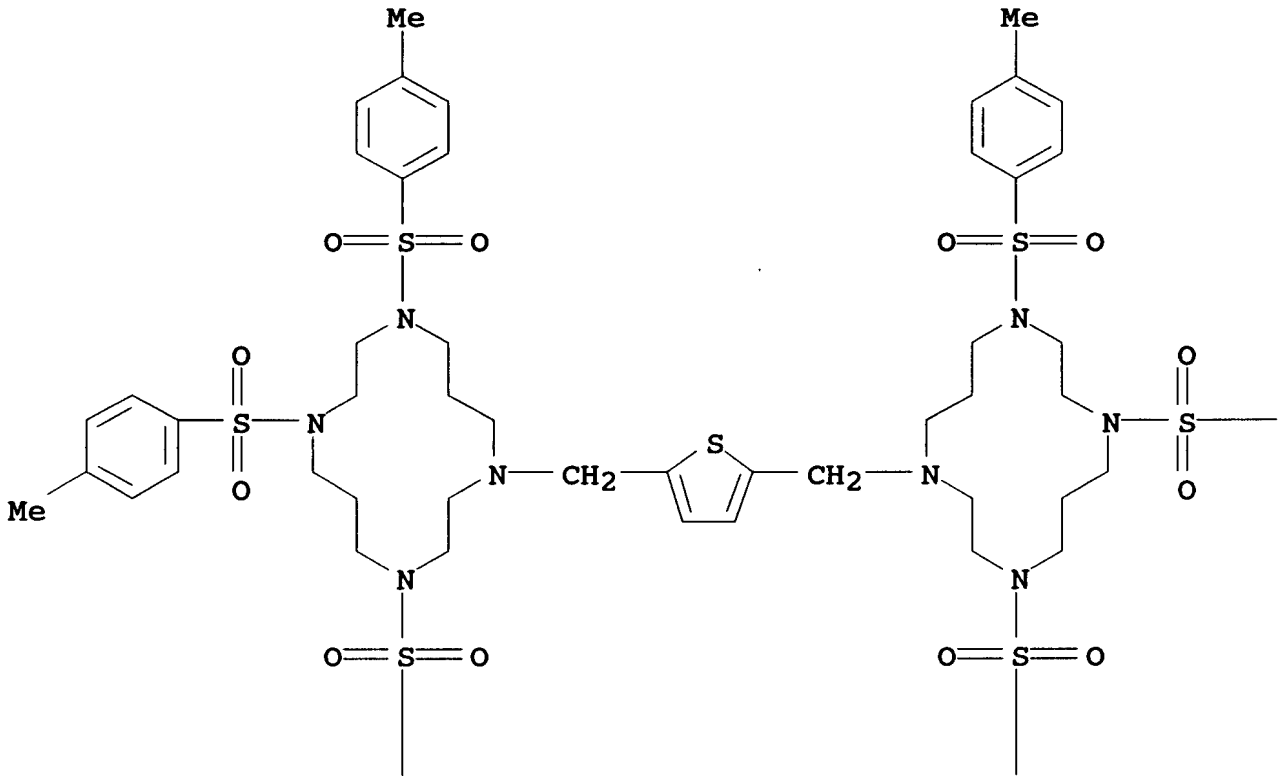
● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

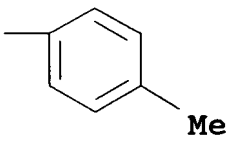
REFERENCE 1: P 120:30786

L46 ANSWER 23 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-16-1 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,5-thiophenediylbis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C68 H88 N8 O12 S7
SR CA
LC STN Files: CA

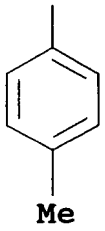
PAGE 1-A

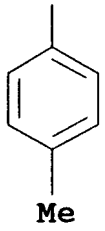


PAGE 1-B



PAGE 2-A

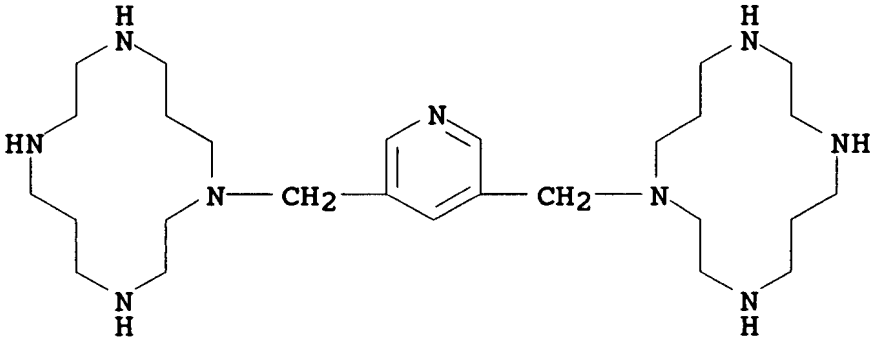




1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 24 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-09-2 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediylbis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H53 N9
CI COM
SR CA
LC STN Files: CA, TOXLIT

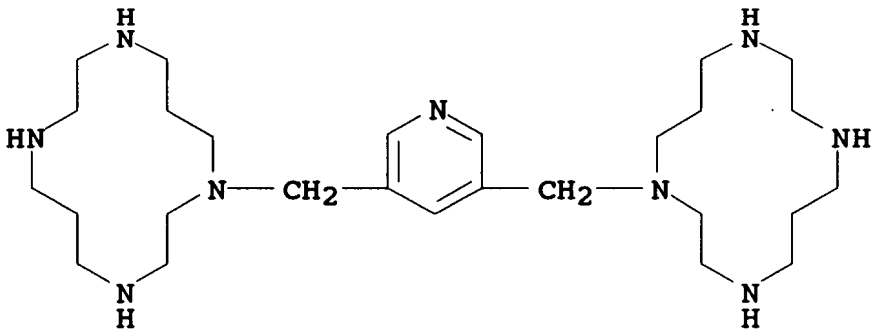


2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

REFERENCE 2: P 120:30786

L46 ANSWER 25 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-08-1 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediylbis(methylene)]bis-, nonahydrobromide (9CI) (CA INDEX NAME)
MF C27 H53 N9 . 9 Br H
SR CA
LC STN Files: CA
CRN (151191-09-2)



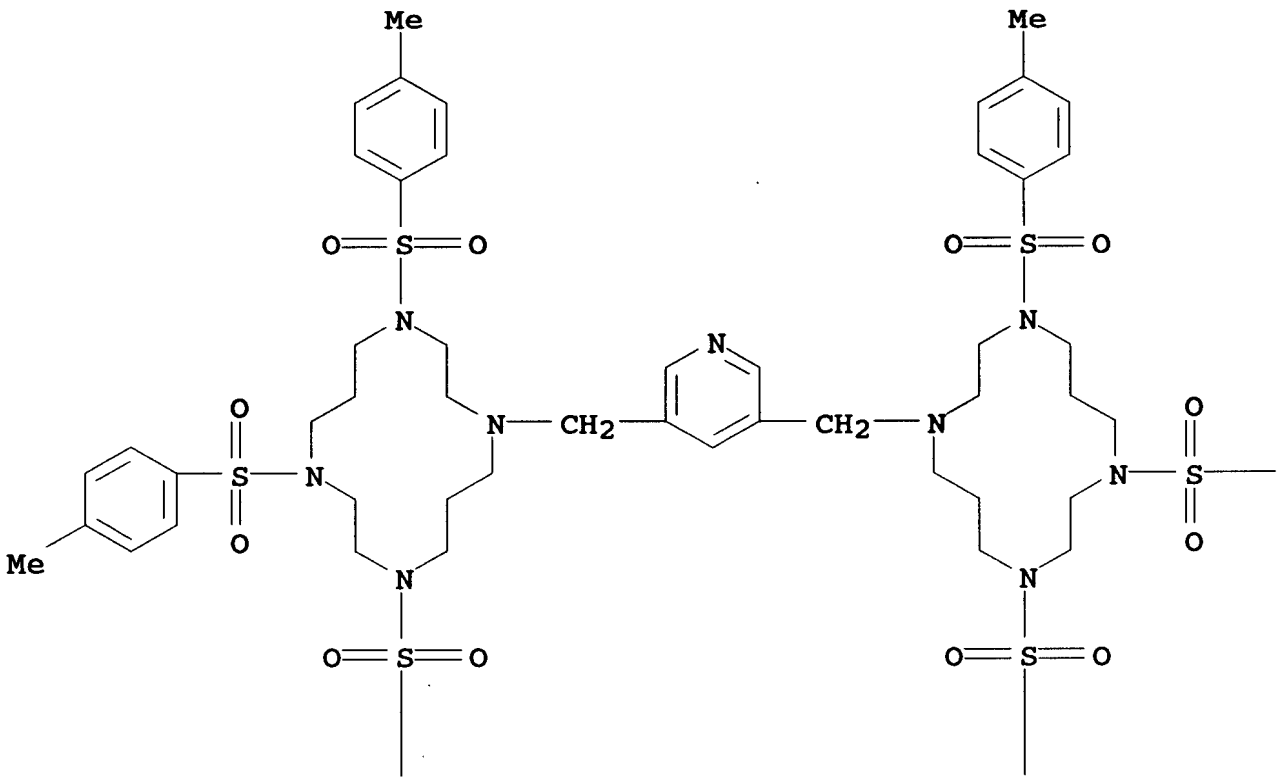
● 9 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

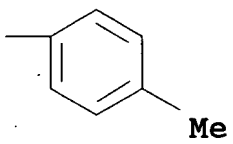
REFERENCE 1: P 120:30786

L46 ANSWER 26 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-07-0 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediylbis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C69 H89 N9 O12 S6
SR CA
LC STN Files: CA

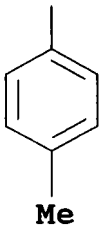
PAGE 1-A

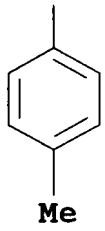


PAGE 1-B



PAGE 2-A

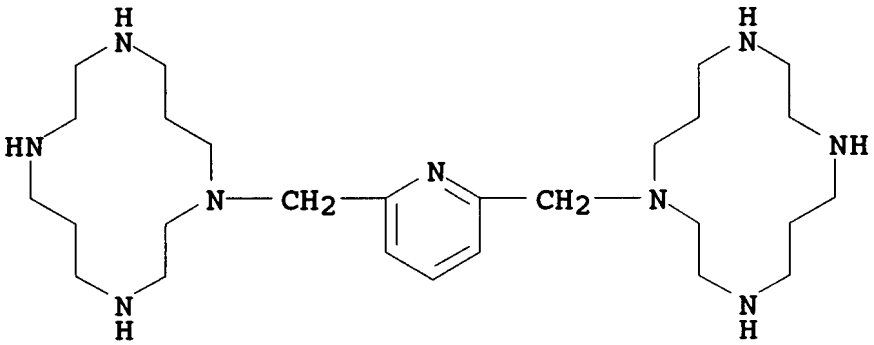




1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 27 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-06-9 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,6-pyridinediylbis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H53 N9
CI COM
SR CA
LC STN Files: CA, TOXLIT

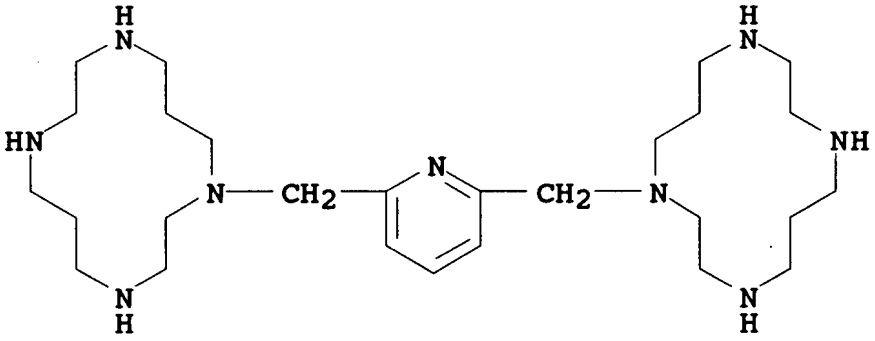


2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

REFERENCE 2: P 120:30786

L46 ANSWER 28 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-05-8 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,6-pyridinediylbis(methylene)]bis-, octahydrobromide (9CI) (CA INDEX NAME)
MF C27 H53 N9 . 8 Br H
SR CA
LC STN Files: CA
CRN (151191-06-9)



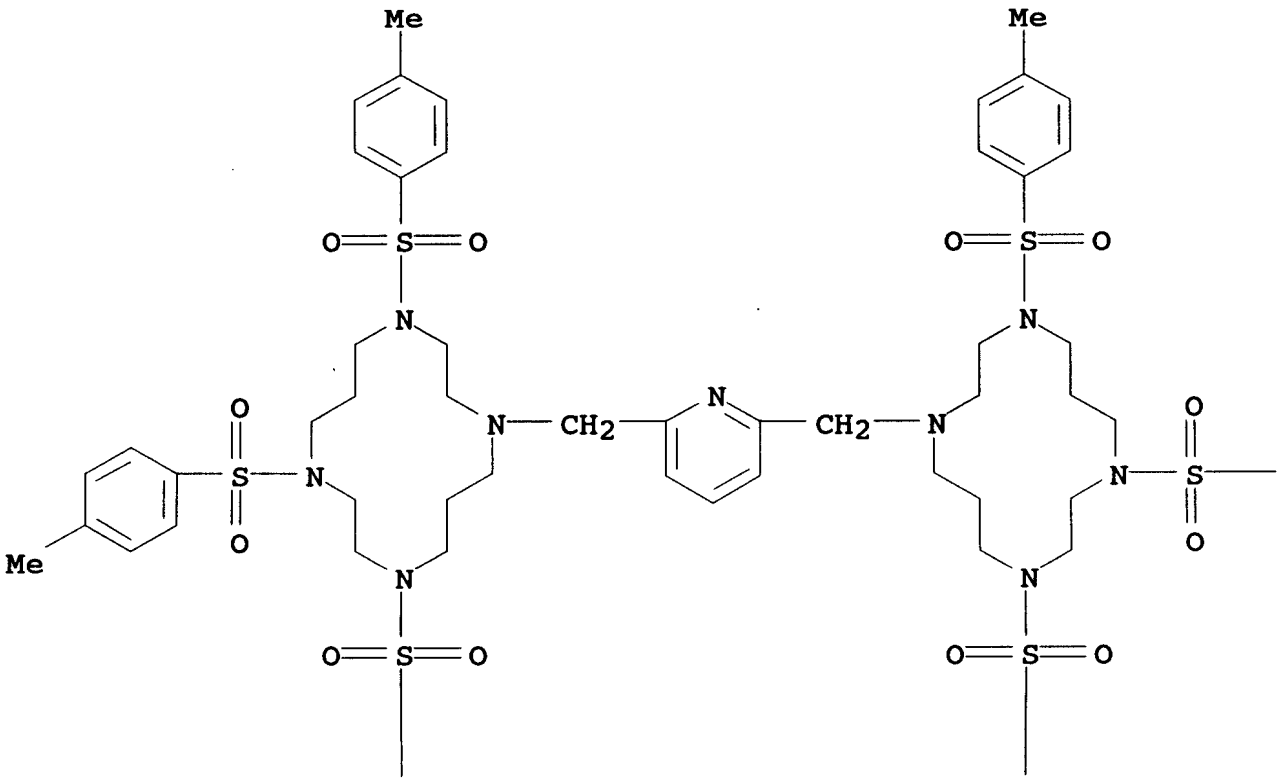
● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

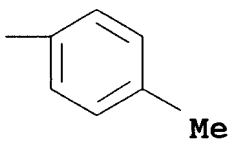
REFERENCE 1: P 120:30786

L46 ANSWER 29 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-04-7 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,6-pyridinediylbis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C69 H89 N9 O12 S6
SR CA
LC STN Files: CA

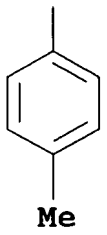
PAGE 1-A

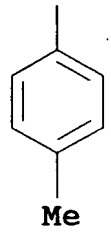


PAGE 1-B



PAGE 2-A

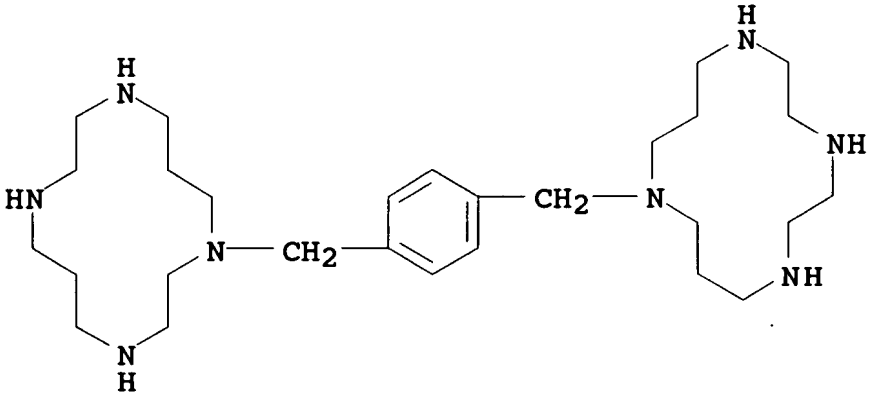




1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 30 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 151191-03-6 REGISTRY
CN 1,4,7,11-Tetraazacyclotetradecane, 11-[[4-(1,4,8,11-tetraazacyclotetradec-1-ylmethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,4,8,11-Tetraazacyclotetradecane, 1,4,7,11-tetraazacyclotetradecane deriv. (9CI)
FS 3D CONCORD
MF C28 H54 N8
CI COM
SR CA
LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

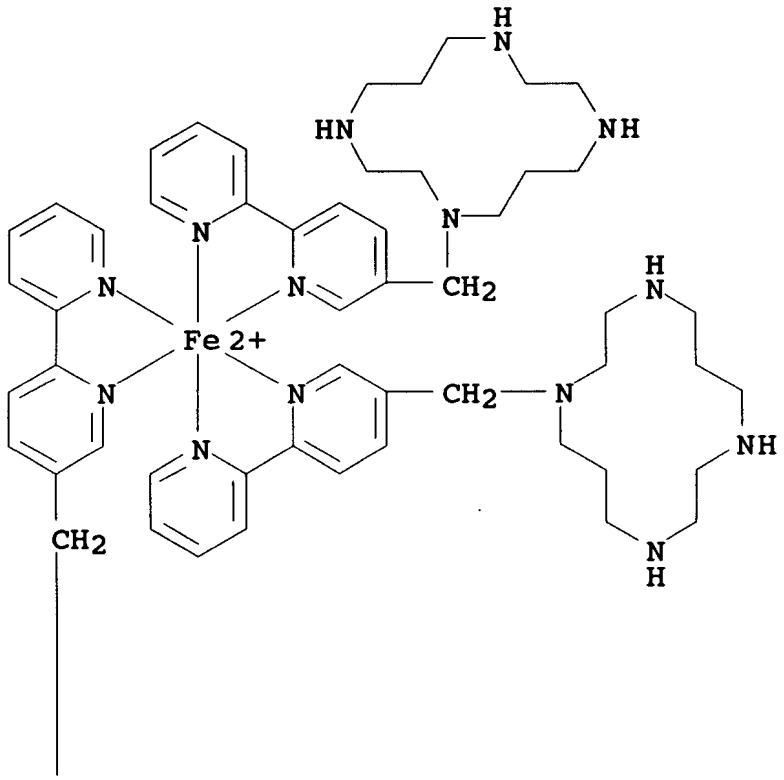
REFERENCE 1: P 120:30786

=> d ide can 50-57

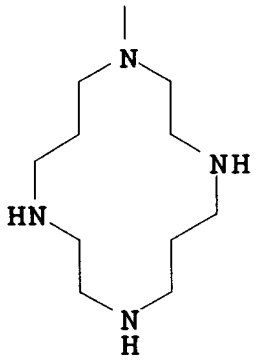
L46 ANSWER 50 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 142079-95-6 REGISTRY
CN Iron(2+), tris[1-([2,2'-bipyridin]-5-ylmethyl)-1,4,8,11-tetraazacyclotetradecane]-, (OC-6-21)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,4,8,11-Tetraazacyclotetradecane, iron(2+) deriv. (9CI)
MF C63 H96 Fe N18

CI CCS
SR CA
LC STN Files: CA
DES 7:OC-6-21

PAGE 1-A



PAGE 2-A

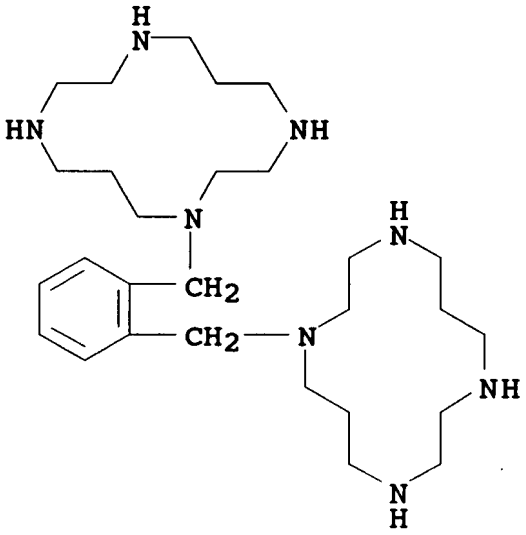


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 117:82274

L46 ANSWER 51 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 133563-60-7 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,2-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8
SR CA
LC STN Files: CA, USPATFULL

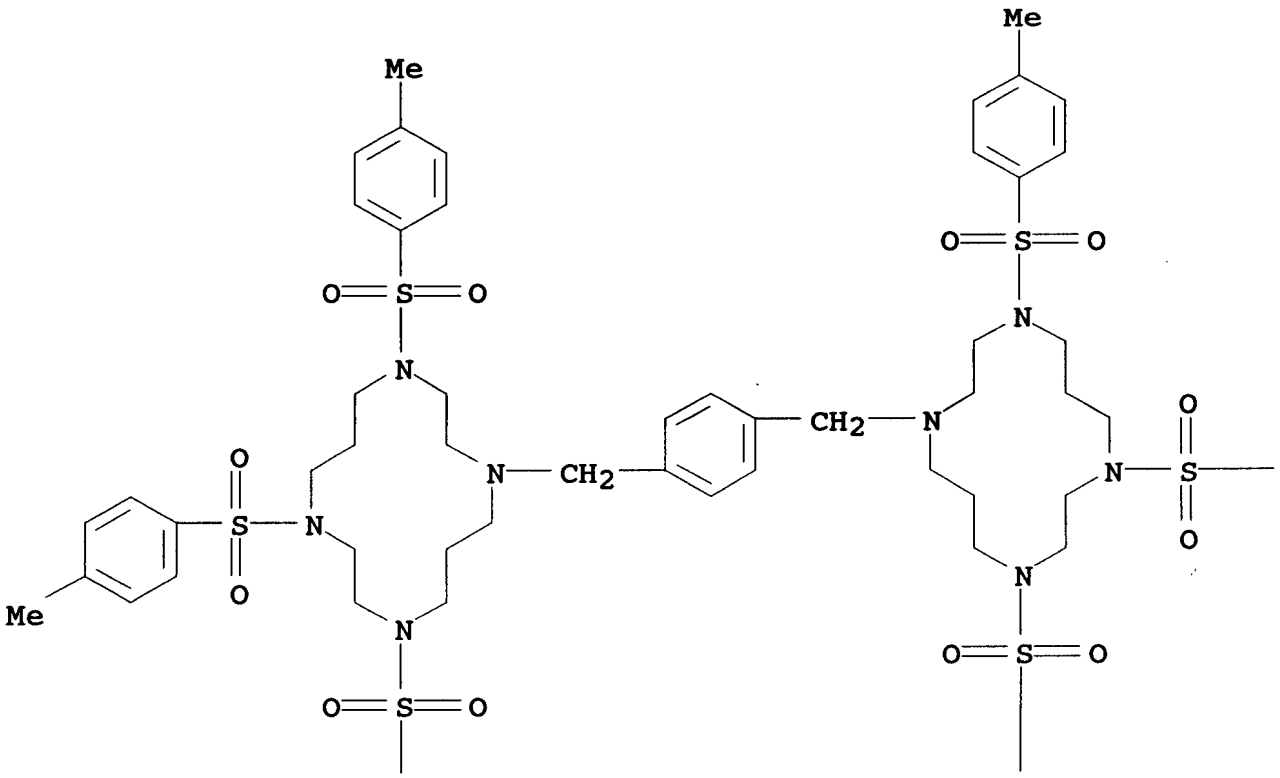


1 REFERENCES IN FILE CA (1967 TO DATE)

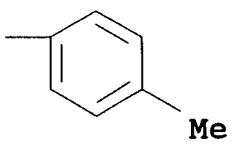
REFERENCE 1: P 114:207294

L46 ANSWER 52 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 110078-47-2 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C70 H90 N8 O12 S6
SR CA
LC STN Files: CA, CJACS

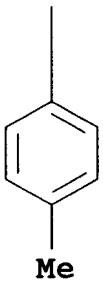
PAGE 1-A

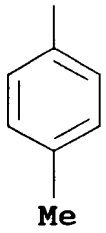


PAGE 1-B



PAGE 2-A

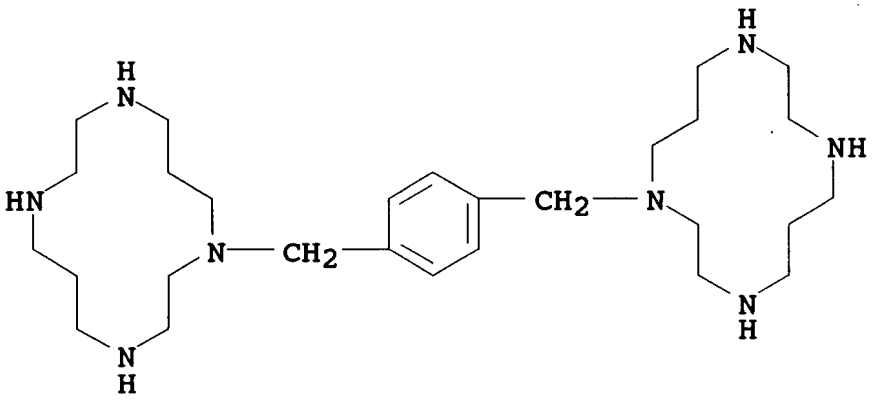




1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 107:167695

L46 ANSWER 53 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 110078-46-1 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8
CI COM
SR CA
LC STN Files: BEILSTEIN*, CA, CJACS, USPATFULL
(*File contains numerically searchable property data)



4 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

REFERENCE 1: P 120:30786

REFERENCE 2: 118:204007

REFERENCE 3: P 114:207294

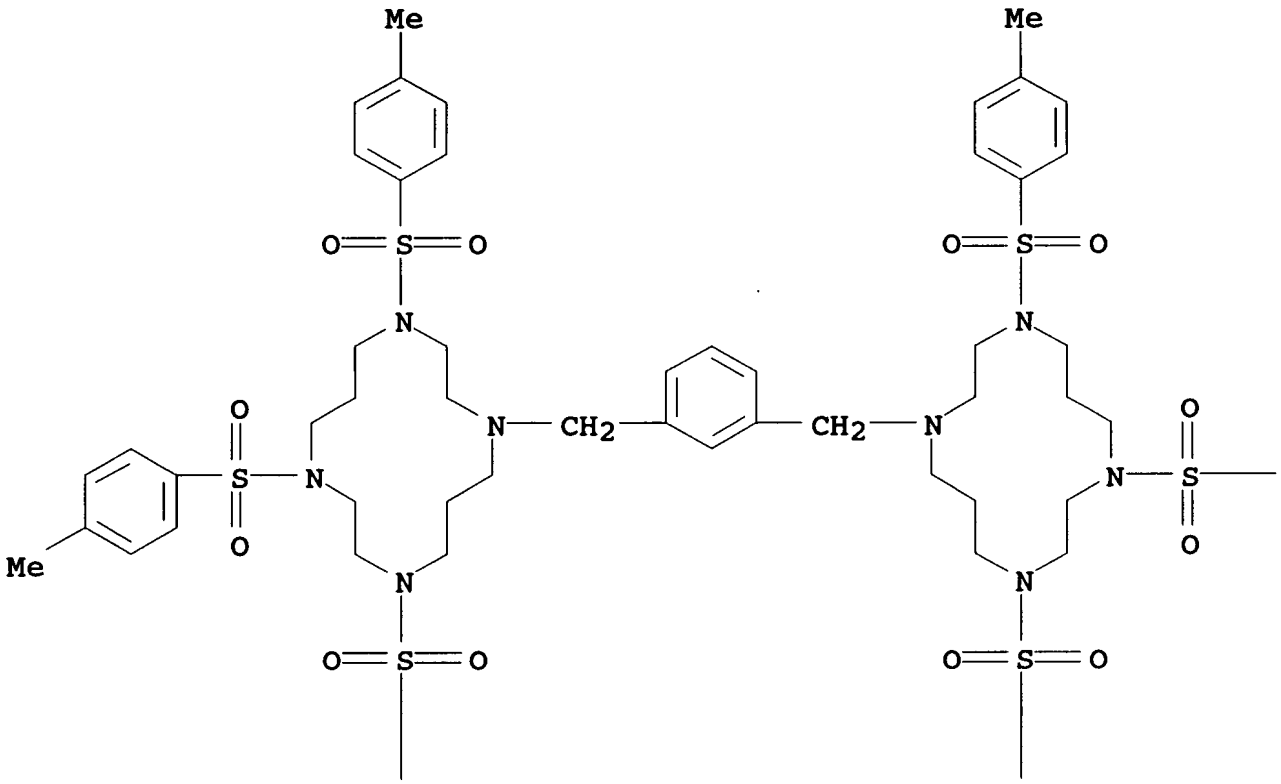
REFERENCE 4: 114:207229

REFERENCE 5: 107:167695

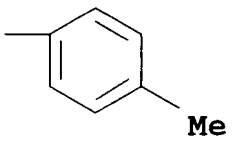
L46 ANSWER 54 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 110078-45-0 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C70 H90 N8 O12 S6
SR CA
LC STN Files: CA, CJACS

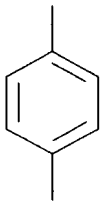
PAGE 1-A

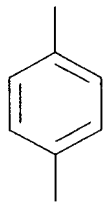


PAGE 1-B



PAGE 2-A

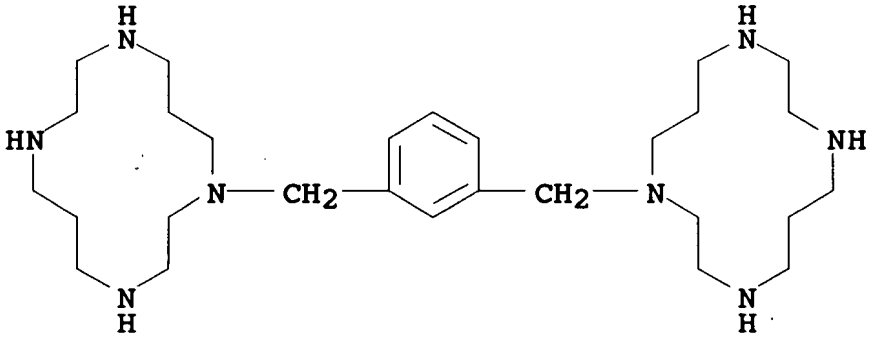




1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 107:167695

L46 ANSWER 55 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 110078-44-9 REGISTRY
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C28 H54 N8
SR CA
LC STN Files: BEILSTEIN*, CA, CHEMINFORMRX, CJACS, TOXLIT, USPATFULL
(*File contains numerically searchable property data)



5 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

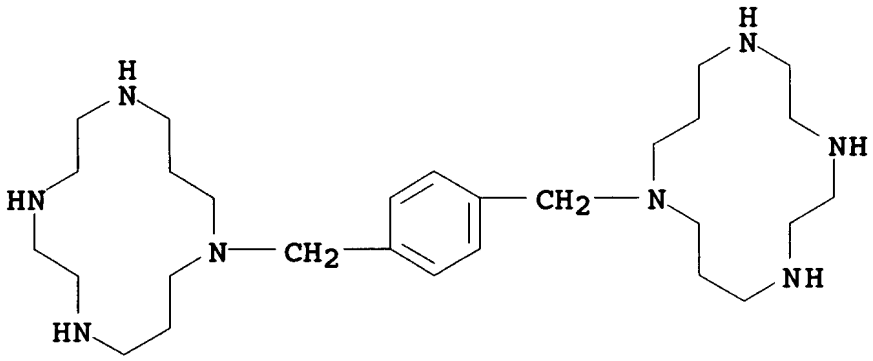
REFERENCE 2: P 120:30786

REFERENCE 3: P 114:207294

REFERENCE 4: 114:207229

REFERENCE 5: 107:167695

L46 ANSWER 56 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 105390-46-3 REGISTRY
CN 1,4,7,11-Tetraazacyclotetradecane, 11,11'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)
MF C28 H54 N8 . 8 Cl H
SR CA
LC STN Files: CA
CRN (151190-99-7)



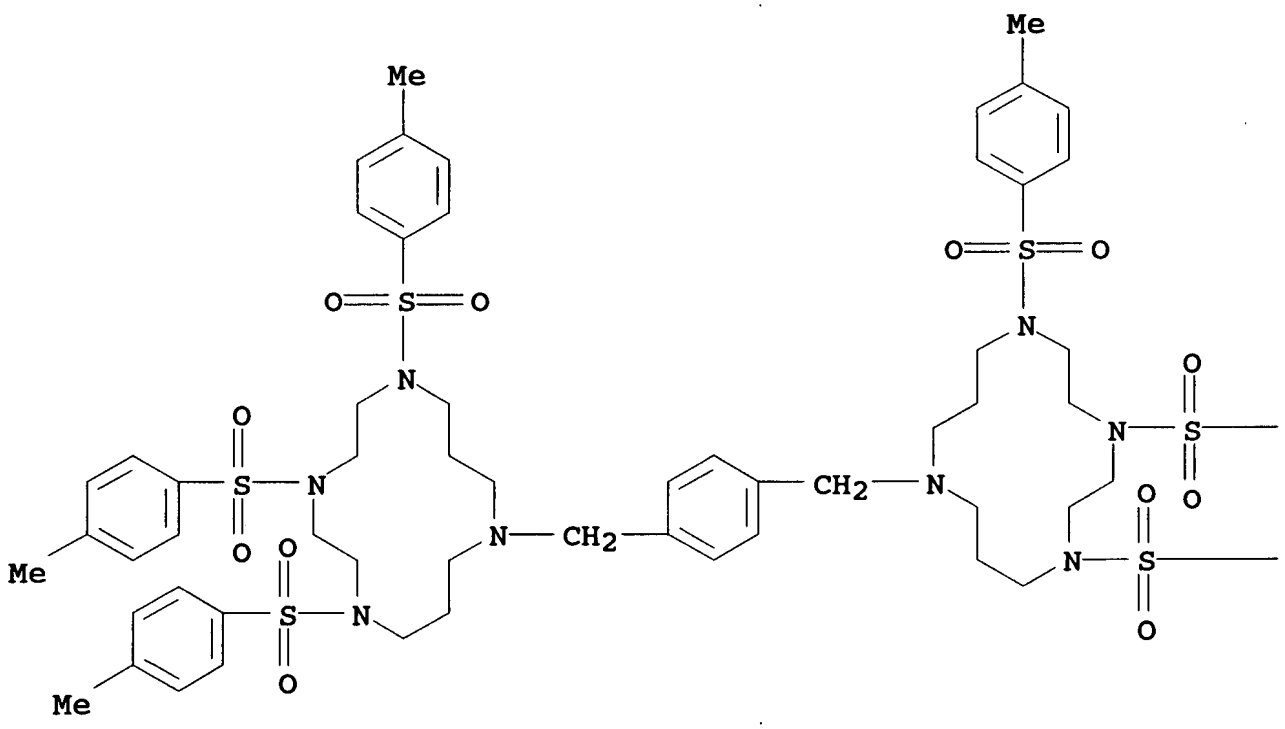
● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

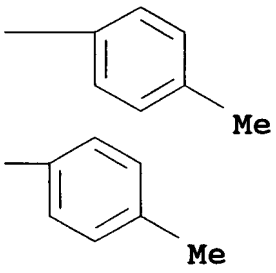
REFERENCE 1: 106:26833

L46 ANSWER 57 OF 57 REGISTRY COPYRIGHT 1995 ACS
RN 105355-16-6 REGISTRY
CN 1,4,7,11-Tetraazacyclotetradecane, 11,11'-[1,4-phenylenebis(methylene)]bis[1,4,7-tris[(4-methylphenyl)sulfonyl]-(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C70 H90 N8 O12 S6
SR CA
LC STN Files: CA

PAGE 1-A



PAGE 1-B



2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

REFERENCE 2: 106:26833

=> fil ca
FILE 'CA' ENTERED AT 14:30:43 ON 25 MAR 95
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE COVERS 1967 - 18 Mar 1995 (950318/ED) VOL 122 ISS 12

To help control your online searching costs, consider using the HCA File when using the FSEARCH command or when conducting SmartSELECT searches with large numbers of terms.

CAPLUS IS NOW ONLINE!

=> s l46
L47 10 L46

=> d 1-10 bib abs hitrn

L47 ANSWER 1 OF 10 CA COPYRIGHT 1995 ACS
AN 121:225706 CA
TI Synthetic Bis-Metal Ion Receptors for Bis-Imidazole "Protein Analogs"
AU Mallik, Sanku; Johnson, Robert D.; Arnold, Frances H.
CS Division of Chemistry and Chemical Engineering 210-41, California Institute of Technology, Pasadena, CA, 91125, USA
SO J. Am. Chem. Soc. (1994), 116(20), 8902-11

CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CJACS-IMAGE; CJACS
AB The authors are investigating an approach to protein recognition that is based on matching a pattern of metal ions in a synthetic receptor to a complementary pattern of metal-coordinating functional groups (histidine) on a protein's surface. In this model study, target "protein analogs" were constructed by linking two imidazoles via org. spacers of varying lengths. By computer modeling the individual targets and receptors,bis-Hg2+ receptors were designed to position two metal ions to match the available nitrogen ligands of their target bis-imidazoles. While 1H NMR studies in DMSO-d6 show that the receptors can bind 2 equiv of 1-benzylimidazole (K1 .apprx. 104 M-1), a bis-imidazole is bound in a 1:1 complex with assocn. consts. as high as 3.times.106 M-1. Bis-metal ion receptors are indeed selective for their target bis-imidazoles in competitive binding expts., preferring the target over others that are both longer and shorter by .apprx.4 .ANG. (max. selectivity = 11.5). A max. selectivity of 140 was obsd. for the competition between a target bis-imidazole and 1-benzylimidazole. Increasing the available coordination sites on the metal ion significantly reduces selectivity, presumably by allowing the receptor to take on multiple bound conformations. Attempts to improve binding selectivity by restricting the receptors' conformational mobility reduced selectivity, primarily by introducing unanticipated unfavorable interactions with the target bis-imidazoles.
IT **147025-65-8P 147025-66-9P 158200-25-0P 158200-26-1P**
(synthetic bis-metal ion receptors for bis-imidazole protein analogs)

L47 ANSWER 2 OF 10 CA COPYRIGHT 1995 ACS
AN 120:289504 CA
TI Highly potent and selective inhibition of human immunodeficiency virus by the bicyclam derivative JM3100
AU De Clerco, Erik; Yamamoto, Naohiko; Pauwels, Rudi; Balzarini, Jan; Witvrouw, Myriam; De Vreese, Karen; Debyser, Zeger; Rosenwirth, Brigitte; Peichl, Peter; et al.
CS Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain, B-3000, Belg.
SO Antimicrob. Agents Chemother. (1994), 38(4), 668-74
CODEN: AMACCQ; ISSN: 0066-4804
DT Journal
LA English
AB Bicyclams, in which the cyclam (1,4,8,11-tetraazacyclotetradecane) moieties are tethered via an aliph. bridge (i.e., propylene, as in JM2763) are potent and selective inhibitors of human immunodeficiency virus type 1 (HIV-1) and type-2 (HIV-2) (E. De Clercq, N. Yamamoto, R. Pauwels, M. Baba, D. Schols, H. Nakashima, J. Balzarini, Z. Debyser, B. A., Murrer, D. Schwartz, D. Thornton, G. Bridger, S. Fricker, G. Henson, M. Abrams, and D. Picker, Proc. Natl. Acad. Sci. USA 89:5286-5290, 1992). The authors have now found that the bicyclam JM3100, in which the cyclam moieties are tethered by an arom. bridge [i.e., phenylenebis(methylene)], inhibits the replication of various HIV-1 and HIV-2 strains in various cell lines at a 50% effective concn. (EC50) of 1 to 10 ng/mL, which is about 100-fold lower than the concn. required for

JM2763 to inhibit HIV replication and at least 100,000-fold lower than the concn. required for JM2763 to inhibit HIV replication and at least 100,000-fold lower than the cytotoxic concn. (>500 .mu.g/mL). In primary T4 lymphocytes or primary monocytes, JM3100 proved inhibitory to HIV-1 (IIIB) and several clin. HIV-1 isolated at an EC50 of less than 1 ng/mL. On the basis of time-of-addn. expts., JM3100 appeared to interact with a viral uncoating event, and this was further corroborated by an uncoating assay in which RNase sensitivity of [5-3H]uridine-labeled virions was monitored. In addn., but possibly mechanistically related, JM3100 blocks formation of infectious particles. JM3100 was also found to interfere directly with virus-induced syncytium formation, albeit at a higher concn. (1 to 2 .mu.g/mL) than that required for inhibition of viral replication. Following s.c. injection of 10 mg of JM3100 per kg of body wt. to rabbits, anti-HIV activity was detected in serum corresponding to serum drug levels exceeding for at least 6 h by >100-fold the EC50 required to inhibit HIV replication in vitro. When combined with either 3'-azido-2',3'-dideoxythymidine or 2',3'-dideoxyinosine, JM3100 achieved a additive inhibition of HIV replication, and when repeatedly subcultivated in the presence of JM3100, the virus remained insensitive to the compd. for at least 30 passages (120 days) in cell culture.

IT **155148-31-5**
(HIV virus inhibition by, mechanism of, structure in relation to, in human cells)

IT **110078-44-9 151191-06-9 151191-09-2 155148-32-6**
(HIV virus inhibition by, structure in relation to, in human cells)

L47 ANSWER 3 OF 10 CA COPYRIGHT 1995 ACS
AN 120:44414 CA
TI Functional group convergency in a binuclear dephosphorylation reagent
AU Vance, David H.; Czarnik, Anthony W.
CS Dep. Chem., Ohio State Univ., Columbus, OH, 43210, USA
SO J. Am. Chem. Soc. (1993), 115(25), 12165-6
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CJACS-IMAGE; CJACS
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Phosphomonoesters experience rapid hydrolysis in the presence of 2 equiv of Co(III) complexes bearing substitutable cis-coordination sites. A binuclear Co(III) complex was synthesized possessing a phosphate-sized pocket, but rigidly so as to avoid .mu.-oxo dimer formation. X-ray anal. of the carbonato form I confirms the cofacial orientation of the metal centers, and 31P NMR of the phosphate complex II suggests triscoordination of phosphate to Co(III). The binuclear complex at 1 mM affects the dephosphorylation of p-nitrophenyl phosphate 10-times faster than do

either the mononuclear Co(III)-cyclen or Co(III)-trpn complexes at 2 mM.

IT **151987-13-2P**
(prepn. and crystal structure and aquation of)
IT **151697-44-8P**
(prepn. and reaction of, with carbonatocobaltate)
IT **151956-64-8P**
(prepn. and reaction with phosphate and catalysis by, of hydrolysis of phosphate esters)

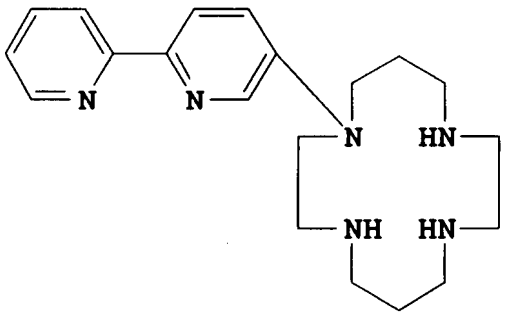
L47 ANSWER 4 OF 10 CA COPYRIGHT 1995 ACS
AN 120:30786 CA
TI Linked heterocyclic polyamines with activity against HIV
IN Bridger, Gary James; Padmanabhan, Sreenivasan; Skerlj, Renato Tony; Thornton, David Michael
PA Johnson Matthey P.L.C., UK
SO PCT Int. Appl., 66 pp.
CODEN: PIXXD2
PI WO 9312096 A1 930624
DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
AI WO 92-GB2334 921216
PRAI GB 91-26677 911216
DT Patent
LA English
OS MARPAT 120:30786
AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 = (un)substituted alk. chain or heteroatom-contg. chain; Y, Z = cyclic polyamine moieties having 9-32 ring members and 3-8 N atoms in the ring spaced by .gtoreq.2 C atoms from each other] or their acid addn. salts or metal complexes are prepd. and demonstrated viricidal activity against HIV-1 and HIV-2. Thus, 1,1'-[1,4-phenylenebis(methylene)]bis-1,4,8,11-tetraazacyclotetradecane was prepd. and demonstrated 50% inhibitory concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory concn. against HIV-2 of <0.01 .mu.g/mL in an assay employing infected MT-4 cells.
IT **151191-32-1 151191-33-2 151191-34-3**
(HIV viricidal activity of)
IT **110078-44-9P 110078-46-1DP**, copper and zinc complexes **151190-72-6P 151190-73-7P 151190-74-8P 151190-75-9P 151190-76-0P 151190-87-3P 151190-93-1P 151190-94-2P 151190-97-5P 151190-98-6P 151190-99-7P 151191-02-5P 151191-03-6P 151191-05-8P 151191-06-9P 151191-08-1P 151191-09-2P 151191-17-2P 151191-18-3P 151191-20-7P 151191-21-8P 151191-26-3P 151191-27-4P 151191-28-5P 151191-29-6P 151191-30-9P 151191-31-0P**
(prepn. and HIV viricidal activity of)
IT **105355-16-6P 151190-70-4P 151190-71-5P 151190-86-2P 151190-92-0P 151191-01-4P 151191-04-7P 151191-07-0P 151191-16-1P 151191-19-4P**
(prepn. and reaction of, in prepn. of heterocyclic HIV viricidal agents)
IT **110078-46-1**

(reaction of, in prepn. of heterocyclic HIV viricidal agents)

L47 ANSWER 5 OF 10 CA COPYRIGHT 1995 ACS
AN 118:204007 CA
TI Selective recognition of bis-imidazoles by complementary bis-metal ion complexes
AU Mallik, Sanku; Johnson, Robert D.; Arnold, Frances H.
CS Div. Chem. Chem. Eng., California Inst. Technol., Pasadena, CA, 91125, USA
SO J. Am. Chem. Soc. (1993), 115(6), 2518-20
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
OS CJACS-IMAGE; CJACS
AB Metal ion complexes capable of selective recognition are made by matching the spatial distribution of metal ions in the complex to the spacing between coordinating ligands on the target mol. Two ligands (L), 1,4-di[(1',4',8',11'-tetraazacyclotetradecan-1'-yl)methylene]benzene (L1) and 2,6-di[(1',4',8',11'-tetraazacyclotetradecan-1'-yl)methylene]naphthalene (L2), were synthesized. The corresponding [Hg2(H2O)L](ClO4) (3) were designed to bind a bis-imidazole target mol., 4,4'-di(imidazol-1-yl)methylenebiphenyl (2), preferentially over the closely related bis-imidazole, 1,4-di(imidazol-1-yl)xylene (1). From 1H NMR chem. shifts in titrn. expts. 3 (L = L1) forms a cyclic complex with 2, but not with 1 in DMSO-d6. Receptor 3 (L = L1) exhibits a selectivity of 10 in binding 2 over 1; the selectivity is increased to 14 with 3 (L = L2). This model system demonstrates that receptor complexes contg. .gtoreq.2 properly-positioned metal ions can selectively bind target mols. with a complementary spatial distribution of metal-coordinating ligands. Metal ion complexes such as these may have applications as synthetic receptors for biol. mols. such as proteins that are characterized by unique pattern of surface coordinating ligands.
IT **110078-46-1DP**, mercury dinuclear complexes with imidazole derivs. **147025-65-8DP**, mercury dinuclear complexes with imidazole derivs.
(formation and binding selectivities of)
IT **147025-66-9P**
(formation and deprotection of)
IT **147025-65-8P**
(prepn. and reaction of, with mercury perchlorate)

L47 ANSWER 6 OF 10 CA COPYRIGHT 1995 ACS
AN 117:82274 CA
TI Synthesis and coordination chemistry of 1-(2',2''-bipyridyl-5'-yl-methyl)-1,4,8,11-tetraazacyclotetradecane L1. Quenching of fluorescence from [Ru(bipy)2(L1)]2+ by coordination of NiII or CuII in the cyclam cavity (bipy = 2,2'-bipyridine; cyclam = 1,4,8,11-tetraazacyclotetradecane)
AU Rawle, Simon C.; Moore, Peter; Alcock, Nathaniel W.
CS Dep. Chem., Univ. Warwick, Coventry, CV4 7AL, UK
SO J. Chem. Soc., Chem. Commun. (1992), (9), 684-7
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CJRSC

GI



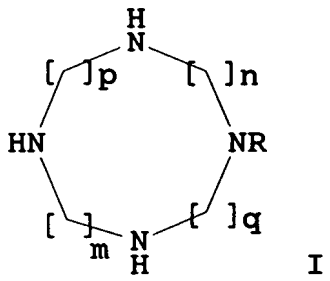
I

AB A novel bipy deriv. (I) of cyclam, designed for controlled and systematic polynuclear metal complex formation, is reported. Fluorescence quenching of the [Ru(bipy)2]2+ core of [(bipy)2RuL]2+ (L = I) upon coordination of CuII at the cyclam cavity is demonstrated. The crystal structure of [CuL](ClO4)2.MeNO2 was detd.

IT **142079-95-6P**
(prepn. of)

L47 ANSWER 7 OF 10 CA COPYRIGHT 1995 ACS
AN 114:207294 CA
TI Preparation of mono-N-substituted cyclic tetramines
IN Handel, Henri; Yaouanc, Jean Jacques; Filali Zegzouti, Ayoub; Malouala, Denis; Des Abbayes, Herve; Clement, Jean Claude; Bernard, Helene; Le Gall, Guenaelle
PA Centre National de la Recherche Scientifique, Fr.
SO Eur. Pat. Appl., 20 pp.
CODEN: EPXXDW
PI EP 389359 A1 900926
DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE
AI EP 90-400762 900320
PRAI FR 89-3600 890320
DT Patent
LA French
OS MARPAT 114:207294
GI

US 5,047,527 X



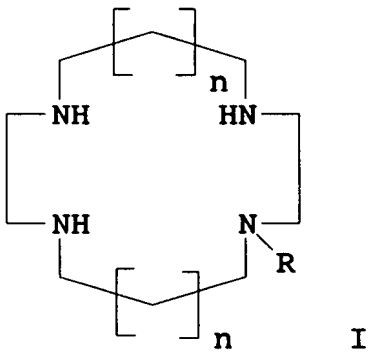
I

AB The title compds. [I; R = (un)satd. org. radical; m-q = 2, 3; m = n = 2 and p = 1 = 3; m = 2 and n-q = 3; n = 2 and m = p = q = 3; m = n

= 3 and p = q = 4] were prepd. by substitution of I (R = H) in which 3 N-atoms are coordinated to a central group, e.g., M(CO)3 (M = Cr, Mo, W). Thus, cyclam was refluxed 2-3 h with Cr(CO)6 in deaerated Bu2O and the product heated 2 h at 100.degree. with PhCH2Br in DMF contg. Na2CO3 to give I (R = PhCH2; m = n = 2, q = 3).

IT **110078-44-9P 110078-46-1P 133563-60-7P**
(prepn. of, method for)

L47 ANSWER 8 OF 10 CA COPYRIGHT 1995 ACS
AN 114:207229 CA
TI Mono N-functionalization of cyclic and linear tetraamines via their tridentate tricarbonylchromium complexes
AU Yaouanc, Jean Jacques; Le Bris, Nathalie; Le Gall, Guenaelle; Clement, Jean Claude; Handel, Henri; Des Abbayes, Herve
CS Fac. Sci. Tech., Brest, 29287, Fr.
SO J. Chem. Soc., Chem. Commun. (1991), (4), 206-7
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CJRSC
GI



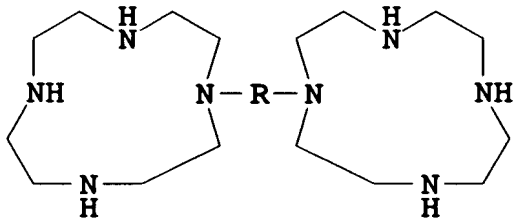
I

AB Cyclic tetraamines I (R = H, n = 0, 1) and H2N(CH2)nNHCH2CH2NH(CH2)nNH2 (n = 2, 3) were selectively monoalkylated in high yield at the uncomplexed N of a Cr(CO)3 tridentate complex. Thus, I (R = H) upon treatment with Cr(CO)6 in Bu2O at 142.degree. gave 85-90% of a tridentate complex, which on treatment with PhCH2Br in DMF at 100.degree. followed by decomplexation afforded 85-95% (R = CH2Ph).

IT **110078-44-9P 110078-46-1P**
(prepn. of, by monoalkylation of tridentate chromium carbonyl complex)

L47 ANSWER 9 OF 10 CA COPYRIGHT 1995 ACS
AN 107:167695 CA
TI Dinickel and dicopper complexes with N,N-linked bis(cyclam) ligands. An ideal system for the investigation of electrostatic effects on the redox behavior of pairs of metal ions
AU Ciampolini, Mario; Fabbrizzi, Luigi; Perotti, Angelo; Poggi, Antonio; Seghi, Barbara; Zanobini, Fabrizio

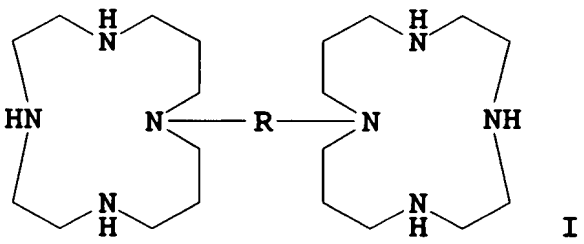
CS Dip. Chim. Gen., Univ. Pavia, Pavia, 27100, Italy
SO Inorg. Chem. (1987), 26(21), 3527-33
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
OS CJACS
GI



I

AB I (R = (CH2)2, (CH2)3, (CH2)4, m-xylyl, p-xylyl) were prepd. by condensation of N,N',N''-tritosylcyclam (2 equiv) with an XRX fragment (X = Br or OTs). M2L4+ (M = Ni, Cu; H4L = I) undergo a 2-electron-oxidn. process, according to 2 reversible 1-electron steps, whose redox potentials are sepd. by the quantity .DELTA.E.degree.. The value of .DELTA.E is related to the comproportionation (or valence scrambling) equil. [MIIIMIIIL]6+ + [MIIMIIL]4+ .dblharw. 2[MIIIMIIL]5+ and results from the combination of a statistical fixed contribution and a term that reflects the electrostatic repulsion between the metal centers of the dinuclear complex. The electrostatic repulsion term decreases when the distance between the metal centers is increased, according to a hyperbolic mode, but does not show any definite dependence upon the macroscopic values of the dielec. const. of the explored media. Moreover, the electrostatic term significantly varies with the stereochem. features of each metal center in its oxidn. state (II or III), which cannot be any longer considered as simple point charges.
IT **110078-45-0P 110078-47-2P**
(prepn. and detosylation of)
IT **110078-44-9P 110078-46-1P**
(prepn. of)

L47 ANSWER 10 OF 10 CA COPYRIGHT 1995 ACS
AN 106:26833 CA
TI Metal complexes with macrocyclic ligands. Part XXII. Synthesis of two bis(tetraaza)macrocycles and study of the structures, electrochemistry, visible and ESR spectra of their binuclear copper(2+) and nickel(2+) complexes
AU Schneider, Rene; Riesen, Andreas; Kaden, Thomas A.
CS Inst. Anorg. Chem., Univ. Basel, Basel, CH-4056, Switz.
SO Helv. Chim. Acta (1986), 69(1), 53-61
CODEN: HCACAV; ISSN: 0018-019X
DT Journal
LA English
GI



I

AB I (R = p-CH2C6H4CH2, CH2CH2) were prepd. by 1,4,7-tritosyl-1,4,7,11-tetraazacyclotetradecane as starting compd. and bifunctional alkylating agents. The bis-macrocycles give binuclear complexes with Ni2+ and Cu2+, the properties of which were studied to obtain information about the interaction of the 2 subunits as a function of the distance. The visible spectra of the Ni2+ and Cu2+ complexes indicate that both metal ions are in a square-planar geometry as expected from the result of the analogous complexes with 1,4,7,11-tetraazacyclotetradecane. Cyclic voltammetry and differential pulse polarog. of the binuclear Ni2+ complexes in CH3CN show a single 2-electron step for I (R = CH2CH2), whereas 2 distinct 1-electron redox processes can be obsd. for I (R = p-CH2C6H4CH2), indicating that the 2 metal ions interact with each other when the chain length is shorter. Similarly, the EPE studies of frozen solns. of the binuclear Cu2+ complexes clearly show that a magnetic dipolar interaction between the 2 paramagnetic centers exists, and that the strength of it depends upon the length of the bridge. Finally, from the x-ray structures of the binuclear Ni2+ complexes with I, 2 rings are kept apart as far as possible; the distances between the two metal ions detd. in the solid correlate well with the observation in soln.

IT **105355-16-6P**
(prepn. and deblocking of)

IT **105390-46-3P**
(prepn. of)